PATENT ABSTRACTS OF JAPAN

(54) MANUFACTURING METHOD AND SYSTEM, DESIGNING METHOD AND STORAGE MEDIUM FOR ELECTRONIC PARTS

(57)Abstract:

PROBLEM TO BE SOLVED: To control a coupling direction of a ferroelectric insulation film, restrict mutual operation with an electric field and restrict a deterioration in an induced electricity due to the electric field, by a method wherein simulation resultants, based on molecular dynamics and fluid models, are utilized for other simulations.

SOLUTION: In a process fluctuation calculation unit I, macro-property not taking into consideration fundamentally an atomic level is calculated, and is stored in a file 2. In file contents, a coupling angle of an interatomic position vector calculated in a molecular dynamics simulation II is inputted to a film characteristic calculation unit III, and a fundamental film characteristic is calculated therein and returned to a file 3. The fundamental film characteristic calculated in the film characteristic calculation unit III is also returned to the process fluctuation calculation unit I as a part of parameters. The molecular dynamics simulation II is executed in combination with a molecular dynamics method and a density function. As a result, it is possible to progress a semiconductor manufacturing process according to a desirable process, or with amendments without a test piece.
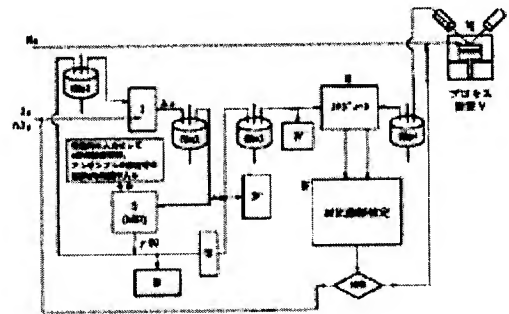
Drawings are not displayable due to the volume of the data (more than 200 drawings).

CLAIMS

[Claim(s)]
[Claim 1]In a simulation method of physical development in a manufacturing installation of a manufacturing process of electronic parts, A manufacturing process factor about the characteristic of an electronic industry material formed in said manufacturing installation is made into an input value, Are prediction data of the characteristic of an electronic industry material which performed a three-dimensional simulation based on this input value, and was formed in a manufacturing installation the method of obtaining, and said simulation, It consists of a process performed based on molecular dynamics, and a process performed based on a fluid model, At least one side of three-dimensional physical quantity outputted as a simulation result performed based on said molecular dynamics and three-dimensional physical quantity outputted as a simulation result performed based on said fluid model, A designing method of a manufacturing process of electronic parts which being transmitted to another side and using for a simulation of a there.
[Claim 2]A designing method of the electronic-parts manufacturing process according to claim 1 characterized by transmitting physical quantity, such as a viscoelasticity coefficient, a Poisson's ratio, a diffusing constant, and Cij, from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model.
[Claim 3]A designing method of the electronic-parts manufacturing process according to claim 1 characterized by transmitting physical quantity, such as a stress tensor, temperature, impurity concentration, and point defect concentration, from a process simulation of said three-dimensional fluid model to said three-dimensional molecular dynamics simulation.
[Claim 4]A designing method of the electronic-parts manufacturing process according to claim 1, wherein said electronic parts are semiconductor devices.
[Claim 5]A designing method of the electronic-parts manufacturing process according to claim 1, wherein it has a stage of inputting fluctuation of said preset value and said molecular dynamics simulation performs variations calculation based on said input value and its fluctuation.
[Claim 6]A designing method of the electronic-parts manufacturing process according to claim 1, wherein said molecular dynamics simulation is performed in combination of a molecular dynamics method and a density functional method.
[Claim 7]A designing method of the electronic-parts manufacturing process according to claim 6, wherein said molecular dynamics method is based on the Takashina round partial differential method.
[Claim 8]A designing method of the electronic-parts manufacturing process according to claim 7, wherein said Takashina round partial differential method is dealing with a three-body problem.
[Claim 9]A designing method of the electronic-parts manufacturing process according to claim 1, wherein said molecular dynamics simulation is performed using experiential potential.
[Claim 10]A designing method of the electronic-parts manufacturing process according to claim 9, wherein said experiential potential is ATTA potential.
[Claim 11]A designing method of the electronic-parts manufacturing process according to claim 9, wherein said experiential potential is BKS potential.
[Claim 12]A process of measuring the characteristic of an electronic industry material formed in a

manufacturing installation in a manufacturing process of electronic parts, and obtaining real observational data, A process of obtaining prediction data of the characteristic of an electronic industry material which made an input value a manufacturing process factor about the characteristic of an electronic industry material formed in said manufacturing installation, performed a three-dimensional simulation based on this input value, and was formed in said manufacturing installation, By a process of carrying out comparison assay of said prediction data and the real observational data, and said comparison assay. When a significant difference is accepted between a preset value of said manufacturing process factor, and said manufacturing process factor guessed from said real observational data, Have a process of carrying out correction processing of said manufacturing process factor, and said simulation, It consists of a process performed based on molecular dynamics, and a process performed based on a fluid model, At least one side of three-dimensional physical quantity outputted as a simulation result performed based on said molecular dynamics and three-dimensional physical quantity outputted as a simulation result performed based on said fluid model, A manufacturing method of electronic parts which being transmitted to another side and using for a simulation of a there.

[Claim 13]A manufacturing method of the electronic parts according to claim 12 a significant difference between said manufacturing process factors guessed from said real observational data having crossed tolerance level, and processing as inferior goods when correction processing is impossible.
[Claim 14]A manufacturing method of the electronic parts according to claim 12 currently carrying out clustering of said manufacturing installation.
[Claim 15]A manufacturing method of the electronic parts according to claim 14, wherein said manufacturing installation which carried out clustering is single wafer processing.
[Claim 16]A manufacturing method of the electronic parts according to claim 12 characterized by transmitting physical quantity, such as a viscoelasticity coefficient, a Poisson's ratio, a diffusing constant, and Cij, from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model.
[Claim 17]A manufacturing method of the electronic parts according to claim 12 characterized by transmitting physical quantity, such as a stress tensor, temperature, impurity concentration, and point defect concentration, from a process simulation of said three-dimensional fluid model to said three-dimensional molecular dynamics simulation.
[Claim 18]A manufacturing method of the electronic parts according to claim 12, wherein said characteristics are a film formed on a semiconductor substrate, a semiconductor substrate surface, and the characteristic about at least one inside a semiconductor substrate.
[Claim 19]A manufacturing method of the electronic parts according to claim 12, wherein comparison assay with said prediction data and real observational data is performed in real time one by one.
[Claim 20]A manufacturing method of the electronic parts according to claim 12, wherein a process of carrying out correction processing of said manufacturing process factor is performed in real time one by one.
[Claim 21]A manufacturing method of the electronic parts according to claim 12, wherein said molecular dynamics simulation is performed in combination of a molecular dynamics method and a density functional method.
[Claim 22]A manufacturing method of the electronic parts according to claim 21, wherein said molecular dynamics method is based on the Takashina round partial differential method.
[Claim 23]A manufacturing method of the electronic parts according to claim 22, wherein said Takashina round partial differential method is dealing with a three-body problem.
[Claim 24]A manufacturing method of the electronic parts according to claim 12, wherein said molecular dynamics simulation is performed using experiential potential.
[Claim 25]A manufacturing method of the electronic parts according to claim 24 characterized by a thing in which said experiential potential is ATTA potential, and to do.
[Claim 26]A manufacturing method of the electronic parts according to claim 24 characterized by a thing in which said experiential potential is BKS potential, and to do.
[Claim 27]A manufacturing method of the electronic parts according to claim 12 characterized by performing a process simulation of a fluid model using at least one prediction data of two or more of said characteristics obtained in said molecular dynamics simulation.

[Claim 28]A manufacturing method of the electronic parts according to claim 27, wherein both said molecular dynamics simulation and a process simulation of a fluid model are three-dimensional simulations.

[Claim 29]A manufacturing method of the electronic parts according to claim 27 characterized by transmitting physical quantity, such as a viscoelasticity coefficient, a Poisson's ratio, a diffusing constant, and Cij, from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model.

[Claim 30]Have the following, and said computer system performs said prediction data and real observational data, and comparison assay by said comparison assay. A manufacturing system of electronic parts characterized by carrying out correction processing of the manufacturing process factor via a control means of said manufacturing installation when a significant difference is accepted between a preset value of said manufacturing process factor, and said manufacturing process factor guessed from said real observational data.

A manufacturing installation of electronic parts.

A measuring device which measures the characteristic of an electronic industry material of said electronic parts formed in said manufacturing installation.

A computer system which makes an input value a preset value of a manufacturing process factor of said electronic parts, performs a simulation based on this input value, and obtains prediction data of said characteristic.

A means to connect said computer system with said measuring device and said manufacturing installation.

[Claim 31]A manufacturing system of the electronic parts according to claim 30 currently carrying out clustering of said manufacturing installation.

[Claim 32]A manufacturing system of the electronic parts according to claim 31, wherein said manufacturing installation which carried out clustering is single wafer processing.

[Claim 33]A manufacturing system of the electronic parts according to claim 30, wherein said simulation is performed based on a molecular dynamics simulation by combination of a molecular dynamics method and a density functional method.

[Claim 34]A manufacturing system of the electronic parts according to claim 30, wherein said characteristics are a film formed on a semiconductor substrate, a semiconductor substrate surface, and the characteristic about at least one inside a semiconductor substrate.

[Claim 35]A manufacturing system of the electronic parts according to claim 30, wherein comparison assay with said prediction data and real observational data is performed in real time one by one.

[Claim 36]A manufacturing system of the electronic parts according to claim 30, wherein a process of carrying out correction processing of said manufacturing process factor is performed in real time one by one.

[Claim 37]A manufacturing system of the electronic parts according to claim 30, wherein fluctuation of said preset value is inputted as said input value and said molecular dynamics simulation performs variations calculation based on said input value and its fluctuation.

[Claim 38]A manufacturing system of the electronic parts according to claim 30, wherein said molecular dynamics method is based on the Takashina round partial differential method.

[Claim 39]A manufacturing system of the electronic parts according to claim 38, wherein said Takashina round partial differential method is dealing with a three-body problem.

[Claim 40]A manufacturing system of the electronic parts according to claim 30, wherein said molecular dynamics simulation uses together a method which used experiential potential.

[Claim 41]A manufacturing system of the electronic parts according to claim 40 characterized by a thing in which said experiential potential is ATTA potential, and to do.

[Claim 42]A manufacturing system of the electronic parts according to claim 40 characterized by a thing in which said experiential potential is BKS potential, and to do.

[Claim 43]A manufacturing system of the electronic parts according to claim 30 characterized by performing a process simulation of a fluid model using at least one prediction data of said characteristic obtained in said molecular dynamics simulation.

[Claim 44]A manufacturing system of the electronic parts according to claim 43, wherein both said

molecular dynamics simulation and a process simulation of a fluid model are three-dimensional simulations.

[Claim 45]A manufacturing system of the electronic parts according to claim 43 characterized by transmitting physical quantity, such as a viscoelasticity coefficient, a Poisson's ratio, a diffusing constant, and Cij, from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model.

[Claim 46]A procedure of inputting a preset value of a manufacturing process factor about the characteristic of an electronic industry material which is a program which performs a simulation of physical development in a manufacturing installation of a manufacturing process of electronic parts, and was formed in said manufacturing installation, A recording medium which recorded a program which performs a procedure of performing a molecular dynamics simulation by combination of a molecular dynamics method and a density functional method based on this input value, and obtaining prediction data of said characteristic and in which computer reading is possible.

[Claim 47]The recording medium according to claim 46, wherein said molecular dynamics simulation is based on combination of a molecular dynamics method and a density functional method.

[Claim 48]The recording medium according to claim 47, wherein said molecular dynamics method is based on the Takashina round partial differential method.

[Claim 49]The recording medium according to claim 48, wherein said Takashina round partial differential method is dealing with a three-body problem.

[Claim 50]The recording medium according to claim 47, wherein said electronic parts are semiconductor devices.

[Claim 51]The recording medium according to claim 47, wherein it has a procedure of inputting fluctuation of said preset value and said molecular dynamics simulation performs variations calculation based on said input value and its fluctuation.

[Claim 52]The recording medium according to claim 47, wherein said molecular dynamics simulation uses together a method which used experiential potential.

[Claim 53]The recording medium according to claim 52 characterized by a thing in which said experiential potential is ATTA potential, and to do.

[Claim 54]The recording medium according to claim 52 characterized by a thing in which said experiential potential is BKS potential, and to do.

[Claim 55]The recording medium according to claim 47 characterized by performing a process simulation of a fluid model using prediction data of said characteristic obtained in said molecular dynamics simulation.

[Claim 56]The recording medium according to claim 55, wherein both said molecular dynamics simulation and a process simulation of a fluid model are three-dimensional simulations.

[Claim 57]The recording medium according to claim 55 characterized by transmitting physical quantity, such as a viscoelasticity coefficient, a Poisson's ratio, a diffusing constant, and Cij, from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model.

[Translation done.]

Drawings are not displayable due to the volume of the data (more than 200 drawings).

DETAILED DESCRIPTION

[Detailed Description of the Invention]
[0001]
[Field of the Invention]This invention relates to the manufacturing method of electronic parts, a manufacturing system, a designing method, and a recording medium, A limited quantity in single wafer processing or the semiconductor device manufacturing installation which carried out clustering, or the "spot" measured value of qualitative contents is especially extended to the maximum, A semiconductor device manufacturing process is related with the manufacturing method of the semiconductor device which makes it possible to go on correcting, the manufacturing system, designing method, and recording medium as a desired process, without using a test piece.
[0002]
[Description of the Prior Art]Conventionally, the manufacturing installation of the semiconductor device has continued up to now through the following changes. If this is looked at in each generation's flow, the generation of dRAM and the chip cost for every generation of the will change, as shown in Drawing 128, while capacity increases from 64K to 256M. The vertical axis of Drawing 128 is expressing the chip cost in 1M as 1. In Drawing 128, the plotted point shows chip cost and the horizontal axis shows the generation of dRAM.
[0003]As shown in Drawing 128, also as for the routing counter, 64K to 256K is comparatively stable, and its chip cost is also stable. Whenever it passes through a generation from 4M, the routing counter is increasing and chip cost is also going up in connection with it. In order to reduce the increase in cost by increase of this routing counter, as shown also in Drawing 128, in 64M. (1) Means, such as standardization [of useless exclusion and (2) work], reduction [of (3) chip sizes], (4) minuteness-making promotion, (5) productivity drive, and (6) FA-ized promotion and formation of (7) large calibers, were provided, and cost reduction is measured.
[0004]If set to 256M, it will put on "Bai" Rule by attaining application of an exotic material, adoption of a high dielectric, application of new structure, solidification, etc. However, if it becomes 1G class, a situation will turn around and will become [whether "Bai" Rule is followed and] unknown. In the conventional method of going in pursuit of highly-efficient-izing of manufacturing installation each to 256M old class to a limit, it becomes difficult to already calculate the solution as an enterprise. It will cause going in pursuit of highly-efficient-izing of manufacturing installation each to a limit, i.e., a high cost.
[0005]As shown in Drawing 129, for every process, from the process A, the device made highly efficient shall be used in order of B->C->D->E->F, and shall go, for example. In this case, it is clear that increase of an equipment field also causes a high cost.
[0006]His not forgetting in more than one more 1G class is that the close control by physical necessity becomes indispensable in each process. For example, they are interception of contamination, exclusion of a natural oxidation film, pursuit of flattening in an atom level, etc. In the present, in consideration of these things, although it is a research stage, the manufacturing installation which carried out clustering as shown in Drawing 130 is proposed as a new concept. This manufacturing installation (cluster tool) that carried out clustering is mainly single wafer processing, although there is also a batch type.

As shown also in Drawing 130, there is a conveyance system in the center, like B->C->D from A, it goes on one by one and each process goes, respectively, as shown in an arrow.
In many cases, it is maintained at a high vacuum, and covering of a natural oxidation film can also decrease, and it has come to be able to perform interception of contamination, and surface control with an atom level within each process and each process at this time.
[0007]On the other hand, vigor and a ferroelectric are going to thin film-ization about the electric field effect MIS element formed on the semiconductor in the technical development of improvement in the speed of these days, and high integration. natural, when a ferroelectrics film is thin-film-ized -- threshold voltage becomes shallow, and main movement speed boils especially AC characteristics markedly by this early, and is made to improve only at this rate If considering EEPROM etc. minuteness making is carried out, it will become a very severe operating condition. In such a case, in the ferroelectrics film of the conventional usual process, sufficient reliability is not acquired any longer.
[0008]However, even if minuteness making of the MIS element is carried out, the remedy of the characteristic of the ferroelectrics film itself is seldom considered, but spends for a high electric field to a gate ferroelectrics film especially in the state where power supply voltage does not fall so much, at the time of main movement. The electron hole generated in impact ionization etc. from channel regions is poured in into a ferroelectrics film by boundary conditions, such as the polarity of a gate electrode, and drain voltage, respectively. And into a ferroelectrics film, the trap of these careers is carried out and it not only reduces long term reliability, but they cause a resisting pressure fall etc.
[0009]It sees with an atom level to a slight degree. In a heat ferroelectrics film, if a high electric field is impressed, for example to a silicon ferroelectrics film, Si-O combination which constitutes a network will interact with the high electric field impressed from the outside. And combination is cut, the trapping center where an electron and an electron hole are captured is formed, it is captured in this trapping center, the field strength distribution of a thickness direction becomes higher than an average electric field locally, and the electron and electron hole through which it passes continuously result in a dielectric breakdown soon.
[0010]It is going to improve these situations, and these days, although the idea which single-crystal-izes a ferroelectrics film was a society level, it began to be advocated. For example, it is reported to J.Appl.Phys., Aol.69 (12), and p8313 (1991) that cerium oxide CeO_2 carries out single crystal growth on a silicon (111) side. Or it is reported to Japan.J.Appl.Phys.Suppl. and Aol.21-1 and p187 (1982) that calcium fluoride CaF2 carries out single crystal growth to silicon single crystal Kami. These are parts. It is not only still in the state of an idea, but the question remains in the calculation technique which becomes a basis of the indicator plentifully.
Then, even if it raises a ferroelectrics film to an example, for example, it is in the situation where the figure of the single crystal of the ferroelectrics film using it itself is not recognized enough one. I will look at what was attached and reported to the structure of this single crystal ferroelectrics film. To one. A. Miyamot, K.Takeichi, T.Hattori, M.Kubo, and T.Inui, "Mechanism of Layer-Layer Homoepitaxial Growth of SrTiO3(100)as Investigated by Molecular Dynamics and Computer Graphics". Jpn. J. Appl. Phys. Vol 31 (1992), There is 4463-4464. Here, stable structure is calculated when pasting it up with a ground Si substrate by using perovskite as a single crystal ferroelectrics film. However, the angle between Ti-Si-Sr and the initial arrangement of distance are accidentally used for Si-O-Ti **. These have simplified the structure of a single crystal ferroelectrics film.
The indicator is not necessarily right.

[0011]If it comes how to design a single crystal ferroelectrics film so that these things may show, the actual condition is almost right being unable to argue. The actual condition is still using the refinement on a formation process from beginning to end about improvement in the characteristic about another side and the ferroelectrics film itself. For example, the purest possible field is prepared beforehand or it is made the argument on the weld slag temperature for film formation, or sputtering ambient from beginning to end. It must be said that these have the still very low recognition including the structure about a single crystal ferroelectrics film or a ferroelectrics film. Since neither the Reason for the spontaneous polarization manifestation of a ferroelectric nor relation with the crystal structure is known, it passes only to phenomenological pursuit.

[0012]
[Problem(s) to be Solved by the Invention]However, in the above new cluster tools, the biggest difficulty faced now is the situation observation technique. That is, in the case of the device which performs single distance, the wafer first called a test piece was introduced into each process. Using this test piece, thickness, a refractive index, etc. were measured and it was being tested whether the process would advance as a predetermined condition.

[0013]There is a problem on quantitative and qualitative understanding in monitoring of the conditions in each cluster tool by use of this test piece. For example, in the stage film formation or the growing process of an oxide film, usually uses the device of XPS or FT-IR. Though this is measured by in-situ, under the present circumstances, the place which the data means cannot fully be examined. It is the judgment grade whether the predetermined substance is generating at most judging from the peak wave number position of the spectrum. There are many places for which it depends on a researcher's judgment in such a situation. Quantitive correspondence cannot be performed and a still more prompt action cannot be performed, either. When there is a strange new substance for which it cannot depend on a researcher's experience, there is no specification of judgment.

[0014]Use of the molecular dynamics simulator is also proposed by one side. however -- comparing a molecular dynamics simulator with a process variation calculation program generally -- (1) -- calculation is dramatically slow and the execution area of the substance made into (2) objects is said to be very small. Then, most of a molecular dynamics simulator and the thing referred to as connecting a process variation calculation program directly was being unable to think. That is, it seemed that the molecular dynamics portion can pull the whole from speed with a late molecular dynamics portion after all, and is not fit for practical use even if it makes it union-ize since calculation is very slow. In a molecular dynamics portion, a calculation area is very small and is about at most tens of A, and on the other hand, since several micron field is calculated, it is difficult in a process variation calculation program, to connect these directly also from a point of a gap of a calculation area.

[0015]For example, this invention persons were kept from forming level in an interface while this energy determined the position and made the highly reliable MIS element by this under impression conditions as installation requirements of a single crystal ferroelectrics film paying attention to the free energy of the whole system including an interface so that it might become the minimum. In searching for the energy of the whole system especially, although it needs to hold strictly and correctly reproducing the structure of a single crystal ferroelectrics film certainly, and how each of these constituted atoms exercise, This invention persons completed ab-initio molecular dynamics, further, in molecular dynamics, established the original potential estimation method, and enabled these calculations for the first time. And it is said that from a meaning to the degree of the quality of a single crystal ferroelectrics film which guarantees improving points, such as an electrical property, enough will be clarified using this.

[0016]For example, combination which constitutes the basic structure of a tunnel insulating film if a high electric field is impressed to a tunnel insulating film. (for example, in the case of a silicon ferroelectrics film, it interacts with Si-O joint), and combination is cut, the electron and electron hole which pass a tunnel insulating film following combination from which it was cut are captured, an electric field becomes larger than an average electric field locally according to the electric charge distribution in a film, and degradation advances further. In order to suppress advance of degradation, according to this invention person, it is suppressing cutting of combination (for example, Si-O combination) of the insulator layer by this electric field.

[0017]It depends for the interaction with combination of an electric field and an insulator layer on direction of an electric field and the direction to combination of an insulator layer. Therefore, in order to weaken an interaction, the direction to combination of an insulator layer is making the thing of strong direction an interaction decrease more. So that amorphously, when completely random, a part of combination of an insulator layer serves as direction with a certainly strong interaction with an electric field.

[0018]The purpose of this invention controls the direction to combination of a ferroelectric insulator layer, suppresses an interaction with an electric field, and aims at aiming at control of dielectric degradation by an electric field.

[0019]This is related with high reliability dielectric film creation art, and this invention person etc. produce it based on the calculation result by the new abinitio molecular dynamics system, and original

experimental data. The single crystal ferroelectrics film can get worse on the contrary than an amorphous dielectric film, if neither a substrate nor physical relationship with a substrate electrode besides selection of the material itself is optimized when this is applied to a ferroelectrics film etc. It is said that the material at this time and the criteria of crystal orientation will be shown. As a new indicator by this invention person, if a word dares to describe, it will be "performing crystal arrangement so that the free energy of a system may become the minimum under a main impressed electric field" etc. "Tolerance level etc. of the crystal defect concentration which may exist in a single crystal ferroelectrics film" is actually described as upper problem. "The tolerance level etc. where the free-energy distribution at the time of seeing locally is uneven in order that the free energy of the system at the time of main impression may deter the trigger of degradation other than the arrangement which becomes the minimum" is described.

[0020]having very complicated structures, such as perovskite symmetrical with 4 times, even if it takes up even a single crystal ferroelectrics film, and the combination of a plane of composition with a substrate — large — the characteristic — things, although things etc. are very complicated, according to this invention person etc., "it gaining" under main movement voltage, even if "it loses" crystallographically — it comes out.

[0021]This invention solves the problem of the monitoring facility in clustering, and A semiconductor device manufacturing installation, A limited quantity especially in single wafer processing or a clustering manufacturing installation or the "spot" measured value of qualitative contents is extended to the maximum, It aims at providing the manufacturing method of the semiconductor device which makes it possible to go on while a request corrects a semiconductor device manufacturing process without a test piece as a process, a manufacturing installation, a simulation method, and a simulator.

[0022]

[Means for Solving the Problem]This invention persons develop a new variations numerical orientation method, using abinitio molecular dynamics, (i) A superposition phenomenon of fluctuation of each process element and a gap of each element was also diagnosed, and a simulation system which also enables a check of whether to perform as a sequence of a (ii) request and discovery of a (iii) change factor was developed. the further feature of this system — change of a (vi) process — mathematical, a point it enabled it to deal with statistically and efficiently, and (v) — a point which added a new inference engine, and (vi) — it is in a point which added a new opposite direction system.

[0023]In a simulation method of physical development in a manufacturing installation of a manufacturing process of electronic parts this invention (Claim 1), A manufacturing process factor about the characteristic of an electronic industry material formed in said manufacturing installation is made into an input value, Are prediction data of the characteristic of an electronic industry material which performed a three-dimensional simulation based on this input value, and was formed in a manufacturing installation the method of obtaining, and said simulation, It consists of a process performed based on molecular dynamics, and a process performed based on a fluid model, At least one side of three-dimensional physical quantity outputted as a simulation result performed based on said molecular dynamics and three-dimensional physical quantity outputted as a simulation result performed based on said fluid model, A simulation method of a manufacturing process of electronic parts which being transmitted to another side and using for a simulation of a there is provided.

[0024]In above-mentioned Claim 1, this invention (Claim 2) from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model. An electronic-parts manufacture process simulation method, wherein physical quantity, such as a viscoelasticity coefficient, a stress constant, a diffusing constant, and Cij, is transmitted is provided.

[0025]In above-mentioned Claim 1, this invention (Claim 3) from a process simulation of said three-dimensional fluid model to said three-dimensional molecular dynamics simulation. An electronic-parts manufacture process simulation method, wherein physical quantity, such as a viscoelasticity coefficient, a stress constant, a diffusing constant, and Cij, is transmitted is provided.

[0026]This invention (Claim 4) provides an electronic-parts manufacture process simulation method, wherein said electronic parts are semiconductor devices in above-mentioned Claim 1.

[0027]In above-mentioned Claim 1, this invention (Claim 5) is further provided with a stage of inputting fluctuation of said preset value, and provides an electronic-parts manufacture process simulation method, wherein said molecular dynamics simulation performs variations calculation based on said input

value and its fluctuation.

[0028]This invention (Claim 6) provides an electronic-parts manufacture process simulation method, wherein said molecular dynamics simulation is performed in combination of a molecular dynamics method and a density functional method in above-mentioned Claim 1.

[0029]This invention (Claim 7) provides an electronic-parts manufacture process simulation method, wherein said molecular dynamics method is based on the Takashina round partial differential method in above-mentioned Claim 6.

[0030]This invention (Claim 8) provides an electronic-parts manufacture process simulation method, wherein said Takashina round partial differential method is dealing with a three-body problem in above-mentioned Claim 7.

[0031]This invention (Claim 9) provides an electronic-parts manufacture process simulation method, wherein said molecular dynamics simulation is performed using experiential potential in above-mentioned Claim 1.

[0032]This invention (Claim 10) provides an electronic-parts manufacture process simulation method characterized by a thing in which said experiential potential is ATTA potential, and to do in above-mentioned Claim 9.

[0033]This invention (Claim 11) provides an electronic-parts manufacture process simulation method characterized by a thing in which said experiential potential is BKS potential, and to do in above-mentioned Claim 9.

[0034]Namely, according to above-mentioned Claim 1 thru/or the electronic-parts manufacture process simulation method according to claim 11. A motion of an atom is anew checked by verifying a finer portion with a process simulation performed [calculation / of process induction stress of an extensive field of several micron level] in a result based on molecular dynamics by a process simulation performed based on a fluid model. More more exact information can be acquired by performing a process simulation of a fluid model again and repeating this if needed.

[0035]A process of this invention (Claim 12) measuring the characteristic of an electronic industry material formed in a manufacturing installation in a manufacturing process of electronic parts, and obtaining real observational data, A process of obtaining prediction data of the characteristic of an electronic industry material which made an input value a manufacturing process factor about the characteristic of an electronic industry material formed in said manufacturing installation, performed a three-dimensional simulation based on this input value, and was formed in said manufacturing installation, By a process of carrying out comparison assay of said prediction data and the real observational data, and said comparison assay. When a significant difference is accepted between a preset value of said manufacturing process factor, and said manufacturing process factor guessed from said real observational data, Have a process of carrying out correction processing of said manufacturing process factor, and said simulation, It consists of a process performed based on molecular dynamics, and a process performed based on a fluid model, At least one side of three-dimensional physical quantity outputted as a simulation result performed based on said molecular dynamics and three-dimensional physical quantity outputted as a simulation result performed based on said fluid model, A manufacturing method of electronic parts of electronic parts which being transmitted to another side and using for a simulation of a there is provided.

[0036]A significant difference between said manufacturing process factors it is guessed from said real observational data in above-mentioned Claim 12 that this inventions (Claim 13) are has crossed tolerance level, When correction processing is impossible, an electronic-parts manufacture process simulation method processing as inferior goods is provided.

[0037]This invention (Claim 14) provides a manufacturing method of electronic parts currently carrying out clustering of said manufacturing installation in above-mentioned Claim 12.

[0038]This invention (Claim 15) provides a manufacturing method of electronic parts, wherein said manufacturing installation which carried out clustering is single wafer processing in above-mentioned Claim 14.

[0039]In above-mentioned Claim 12, this invention (Claim 16) from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model. An electronic-parts manufacture process simulation method, wherein physical quantity, such as a viscoelasticity coefficient, a stress constant, a diffusing constant, and Cij, is transmitted is provided.

[0040]In above-mentioned Claim 12, this invention (Claim 17) from a process simulation of said three-dimensional fluid model to said three-dimensional molecular dynamics simulation. An electronic-parts manufacture process simulation method, wherein physical quantity, such as a viscoelasticity coefficient, a stress constant, a diffusing constant, and Cij, is transmitted is provided.

[0041]This invention (Claim 18) provides a manufacturing method of electronic parts, wherein said characteristics are a film formed on a semiconductor substrate, a semiconductor substrate surface, and the characteristic about at least one inside a semiconductor substrate in above-mentioned Claim 12.

[0042]This invention (Claim 19) provides a manufacturing method of electronic parts, wherein comparison assay with said prediction data and real observational data is performed in real time one by one in above-mentioned Claim 12.

[0043]This invention (Claim 20) provides a manufacturing method of electronic parts, wherein a process of carrying out correction processing of said manufacturing process factor is performed in real time one by one in above-mentioned Claim 12.

[0044]This invention (Claim 21) provides a manufacturing method of electronic parts, wherein said molecular dynamics simulation is performed in combination of a molecular dynamics method and a density functional method in above-mentioned Claim 12.

[0045]This invention (Claim 22) provides a manufacturing method of electronic parts, wherein said molecular dynamics method is based on the Takashina round partial differential method in above-mentioned Claim 21.

[0046]This invention (Claim 23) provides a manufacturing method of electronic parts, wherein said Takashina round partial differential method is dealing with a three-body problem in above-mentioned Claim 22.

[0047]This invention (Claim 24) provides a manufacturing method of electronic parts, wherein said molecular dynamics simulation is performed using experiential potential in above-mentioned Claim 12.

[0048]This invention (Claim 25) provides a manufacturing method of electronic parts characterized by a thing in which said experiential potential is ATTA potential, and to do in above-mentioned Claim 24.

[0049]This invention (Claim 26) provides a manufacturing method of electronic parts characterized by a thing in which said experiential potential is BKS potential, and to do in above-mentioned Claim 24.

[0050]This invention (Claim 27) provides a manufacturing method of electronic parts, wherein a process simulation of a fluid model is performed in above-mentioned Claim 12 using at least one prediction data of two or more of said characteristics obtained in said molecular dynamics simulation.

[0051]This invention (Claim 28) provides a manufacturing method of electronic parts, wherein both said molecular dynamics simulation and a process simulation of a fluid model are three-dimensional simulations in above-mentioned Claim 27.

[0052]In above-mentioned Claim 27, this invention (Claim 29) from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model. A manufacturing method of electronic parts, wherein physical quantity, such as a viscoelasticity coefficient, a stress constant, a diffusing constant, and Cij, is transmitted is provided.

[0053]Namely, according to the manufacturing method of above-mentioned Claim 12 thru/or the electronic parts according to claim 29. Calculation of process induction stress of an extensive field of several micron level with a process simulation performed based on a fluid model a result, A motion of an atom is checked anew, calculating a correction amount of a physical property value by verifying a finer portion with a process simulation performed based on molecular dynamics. Therefore, a check of whether to perform as a desired sequence and discovery of a change factor are also attained, performing diagnosis in real time.

[0054]A measuring device with which this invention (Claim 30) measures a manufacturing installation of electronic parts, and the characteristic of an electronic industry material of said electronic parts of having been formed in said manufacturing installation, A computer system which makes an input value a preset value of a manufacturing process factor of said electronic parts, performs a simulation based on this input value, and obtains prediction data of said characteristic, Have a means to connect said computer system with said measuring device and said manufacturing installation, and said computer system, Perform said prediction data and real observational data, and comparison assay by said comparison assay. When a significant difference is accepted between a preset value of said manufacturing process factor, and said manufacturing process factor guessed from said real

observational data, a manufacturing system of electronic parts carrying out correction processing of the manufacturing process factor via a control means of said manufacturing installation is provided.

[0055]This invention (Claim 31) provides a manufacturing system of electronic parts currently carrying out clustering of said manufacturing installation in above-mentioned Claim 30.

[0056]This invention (Claim 32) provides a manufacturing system of electronic parts, wherein said manufacturing installation which carried out clustering is single wafer processing in above-mentioned Claim 31.

[0057]This invention (Claim 33) provides a manufacturing system of electronic parts, wherein said simulation is performed based on a molecular dynamics simulation by combination of a molecular dynamics method and a density functional method in above-mentioned Claim 30.

[0058]This invention (Claim 34) provides a manufacturing system of electronic parts, wherein said characteristics are a film formed on a semiconductor substrate, a semiconductor substrate surface, and the characteristic about at least one inside a semiconductor substrate in above-mentioned Claim 30.

[0059]This invention (Claim 35) provides a manufacturing system of electronic parts, wherein comparison assay with said prediction data and real observational data is performed in real time one by one in above-mentioned Claim 30.

[0060]This invention (Claim 36) provides a manufacturing system of electronic parts, wherein a process of carrying out correction processing of said manufacturing process factor is performed in real time one by one in above-mentioned Claim 30.

[0061]In above-mentioned Claim 30, further, fluctuation of said preset value is inputted as said input value, and this invention (Claim 37) provides a manufacturing system of electronic parts, wherein said molecular dynamics simulation performs variations calculation based on said input value and its fluctuation.

[0062]This invention (Claim 38) provides a manufacturing system of electronic parts, wherein said molecular dynamics method is based on the Takashina round partial differential method in above-mentioned Claim 30.

[0063]This invention (Claim 39) provides a manufacturing system of electronic parts, wherein said Takashina round partial differential method is dealing with a three-body problem in above-mentioned Claim 38.

[0064]This invention (Claim 40) provides a manufacturing system of electronic parts, wherein said molecular dynamics simulation uses together a method which used experiential potential in above-mentioned Claim 30.

[0065]This invention (Claim 41) provides a manufacturing system of electronic parts characterized by a thing in which said experiential potential is ATTA potential, and to do in above-mentioned Claim 40.

[0066]This invention (Claim 42) provides a manufacturing system of electronic parts characterized by a thing in which said experiential potential is BKS potential, and to do in above-mentioned Claim 40.

[0067]This invention (Claim 43) provides a manufacturing system of electronic parts, wherein a process simulation of a fluid model is performed in above-mentioned Claim 30 using at least one prediction data of said characteristic obtained in said molecular dynamics simulation.

[0068]This invention (Claim 44) provides a manufacturing system of electronic parts, wherein both said molecular dynamics simulation and a process simulation of a fluid model are three-dimensional simulations in above-mentioned Claim 43.

[0069]In above-mentioned Claim 43, this invention (Claim 45) from said three-dimensional molecular dynamics simulation to a process simulation of said three-dimensional fluid model. A manufacturing system of electronic parts, wherein physical quantity, such as a viscoelasticity coefficient, a stress constant, a diffusing constant, and Cij, is transmitted is provided.

[0070]That is, according to the manufacturing system of above-mentioned Claim 30 thru/or the electronic parts according to claim 45, it becomes possible to predict various physical problems in real time as a diagnostic tool in real time by a simulation by a computer.

[0071]A procedure of inputting a preset value of a manufacturing process factor about the characteristic of an electronic industry material which this invention (Claim 46) is a program which performs a simulation of physical development in a manufacturing installation of a manufacturing process of electronic parts, and was formed in said manufacturing installation, A molecular dynamics simulation by combination of a molecular dynamics method and a density functional method is

performed based on this input value, and a recording medium which recorded a program which performs a procedure of obtaining prediction data of said characteristic and in which computer reading is possible is provided.

[0072]This invention (Claim 47) provides a recording medium, wherein said molecular dynamics simulation is based on combination of a molecular dynamics method and a density functional method in above-mentioned Claim 46.

[0073]This invention (Claim 48) provides a recording medium, wherein said molecular dynamics method is based on the Takashina round partial differential method in above-mentioned Claim 47.

[0074]This invention (Claim 49) provides a recording medium, wherein said Takashina round partial differential method is dealing with a three-body problem in above-mentioned Claim 48.

[0075]This invention (Claim 50) provides a recording medium, wherein said electronic parts are semiconductor devices in above-mentioned Claim 47.

[0076]In above-mentioned Claim 47, this invention (Claim 51) is further provided with a procedure of inputting fluctuation of said preset value, and provides a recording medium, wherein said molecular dynamics simulation performs variations calculation based on said input value and its fluctuation.

[0077]This invention (Claim 52) provides a recording medium, wherein said molecular dynamics simulation uses together a method which used experiential potential in above-mentioned Claim 47.

[0078]This invention (Claim 53) provides a recording medium characterized by a thing in which said experiential potential is ATTA potential, and to do in above-mentioned Claim 52.

[0079]This invention (Claim 54) provides a recording medium characterized by a thing in which said experiential potential is BKS potential, and to do in above-mentioned Claim 52.

[0080]This invention (Claim 55) provides a recording medium, wherein a process simulation of a fluid model is performed in above-mentioned Claim 47 using prediction data of said characteristic obtained in said molecular dynamics simulation.

[0081]This invention (Claim 56) provides a recording medium, wherein both said molecular dynamics simulation and a process simulation of a fluid model are three-dimensional simulations in above-mentioned Claim 55.

[0082]This invention (Claim 57) provides a recording medium, wherein physical quantity, such as a viscoelasticity coefficient, a stress constant, a diffusing constant, and Cij, is transmitted to a process simulation of said three-dimensional fluid model from said three-dimensional molecular dynamics simulation in above-mentioned Claim 55.

[0083]That is, without the ability of actually working a process unit to also write special preparation and expense according to above-mentioned Claim 46 thru/or the recording medium according to claim 57, a virtual semiconductor manufacturing system can be built and process-simulation ***** can be performed to an inside of a computer. For example, it becomes possible about looking for a new material easily and effectively moreover by conducting a thought experiment using various molecular structure models, and predicting the characteristic of a device using it.

[0084]This invention (Claim 9) by a molecular dynamics simulator which gave an abinitio molecular dynamics process simulator or experiential potential. . It can set to at least one of two or more of the processes of a manufacturing process of a semiconductor device. At least one preset value of two or more manufacturing process factors and fluctuation of this preset value are made into an input value, A film which performed variations calculation based on this input value, and was formed in a manufacturing installation in at least one of said two or more of the processes, A means to obtain a film formed on a semiconductor substrate, a semiconductor substrate surface, and at least one prediction data of two or more characteristics related with at least one inside a semiconductor substrate, Comparison assay of the real observational data produced by measuring at least one of said two or more of the characteristics in at least one of this prediction data and said two or more of the processes is carried out in real time one by one, A simulator which diagnoses and judges a manufacturing process factor possessing a means to perform diagnosis and a judgment of said manufacturing process factor of a semiconductor device is provided.

[0085]A very problem that this invention persons described above about a molecular dynamics simulator on the other hand that calculation is slow, And an execution area of the target substance was able to introduce and conquer a respectively new idea to a problem that it is very small, was able to make a molecular dynamics simulator and a process variation calculation program have been able to unite by a

new method, and, moreover, was able to pull out the new function which is not until now with this union. It explains in order below.

[0086]It touches somewhat in detail about a problem of calculation speed of (1) first. In molecular dynamics, so to speak, according to Newtonian mechanics, the equation of motion is stood, this is allied over 100 pieces or all 1000 atoms to which its attention is paid, and it solves about an atomic piece piece.

[0087]Calculation of power which becomes a basis of this equation of motion is the most complicated. This is the late reason by the conventional calculation technique. Each atom has received power from an atom around it. Power is got also from a long distance atom also from a nearby atom. It is necessary to take this into consideration. It asks for potential energy V_{ij} generally drawn according to a formula of TERESOFU, and based on this, power is computed and it goes. However, the technique of making a table for every direction from the former in general about power in which potential is beforehand added to each atom based on distance, a direction, etc. was taken. About 100 pieces or the 1000 above-mentioned atoms, with reference to a table, a potential size is seen and it goes by this method each time. This takes time dramatically. Power cannot be computed and inclination to each direction of a potential size changes from potential [itself] to power of each direction (refer to drawing 2). Because of this, it turns out that it takes time of a computer dramatically.

[0088]It is because the formula showing potential shape is dramatically complicated as to why it makes a number table to this appearance. As stated also above, an angle (theta) with a mutual position of a surrounding atom, distance (r) of potential (V), etc. are entangled intricately. It is dramatically difficult to differentiate this, therefore this mathematically and to make a function. For example, although theta is a function of r, a surroundings time grows into a function of r again.

[0089]Generally it was dramatically complicated and this invention persons created the new Takashina round partial differential type conventionally in a portion by which partial differential was not tried about such a case so that an argument of an expression potential as mentioned above may go round. thereby, although modification of the formula itself becomes apparently very complicated, calculation is burned very much -- it came to be able to do It is necessary to have ceased to refer to a table like before.

[0090]The first concept of this Takashina round partial differential type is shown below. Generally this is considered supposing three atoms. Namely, if three atoms are generally described, the rest extends this technique and should just go. If there are three atoms, distance with each atom, an angle between the atom to which its attention is paid, etc. are computable. By these, potential can be searched for uniquely and potential "inclination" can be easily computed in any direction based on this. This invention persons were making a partial differential type altogether about a variable patrolled and used, allying these, and solving, were right and checked that a differentiated type was made.

[0091]An outline of a system by this invention is explained concretely below. First, the actual condition of application of this invention is explained with reference to drawing 1. That is, process unit V is some semiconductor manufacturing systems which are actually working. Here, an absorption-of-light spectrum is seen by spectrum meter VI.

[0092]An absorption-of-light spectrum acquired by spectrum meter VI is once stored as the file 4, and is sent to the scheduler VII. A predicted value by this invention mentioned later is also inputted into the scheduler VII, and these are compared with it by the contrast diagnostic assay part IV.

[0093]If a comparison result in the contrast diagnostic assay part IV is over an acceptable value, it will be removed from a line as what does not fill spec. If it is filling, a part for the change will be sent to the process variation calculation unit I as an inference engine.

[0094]In the process variation calculation unit 1, broad view character which is not fundamentally taken into consideration to an atom level is calculated, and it stores in the file 2. As for the contents of the file 2, a position vector between atoms and a bond angle are computed by the molecular dynamics simulator II.

[0095]It is inputted into the membrane-characteristics calculation unit III, basic membrane characteristics are computed here, and a position vector between atoms and a bond angle which were computed by the molecular dynamics simulator II are returned to the file 3. Basic membrane characteristics computed in the membrane-characteristics calculation unit III are returned to the process variation calculation unit I, and let them be a part of a parameter.

[0096]Thus, a manufacturing method of a semiconductor device which makes it possible to go on by this invention while a request corrects a semiconductor device manufacturing process without a test piece as a process is realized.

[0097]The contents of the molecular dynamics simulator II are important especially actually. As shown in a block diagram of drawing 7, specifically, it consists of two portions. The 1st portion IIa uses the Takashina round partial differential method introduced by this artificer, and the 2nd portion IIb conducts analysis in consideration of a high order paragraph more than Miyoshi. Details of analysis in consideration of the Takashina round partial differential method or a high order paragraph more than Miyoshi are explained one by one henceforth.

[0098]That is, this invention persons developed art which also predicts various spectra by a new computational chemistry theory while they left and returned to pure mathematics theory and established a new variations numerical orientation method. Hereafter, the new abinitio molecular motion study in this invention is explained.

[0099]An entire configuration of the new simulation which this invention person etc. developed is shown in drawing 3. The new technique of having compounded a molecular dynamics portion (MD) and a density functional (DFT) was proposed. Proper use with a molecular dynamics method and a density functional method by this invention persons is shown below first, using drawing 3.

[0100]As shown in drawing 3, a molecular dynamics (MD) portion occupied a lower half of a flow chart, and a density functional portion (DFT) occupies an upper half. a molecular dynamics method does not come out OK -- the so-called a little big system in limited temperature is treated, and potential beforehand searched for from the ultimate cause is used for potential between atoms (ion). On the other hand, a density functional (DFT) was made to use, when searching for a ground state of a small system. And naturally a portion of DFT set temperature to 0K. It asked for a potential portion from a ground state of an electron system. A wave function (KS equation) was specifically solved and a partial density functional was used together.

[0101]In a DFT portion, it places in quest of total energy of a ground state of an electron system without degeneracy. Total energy is functional [of electron density (** which does not go back to wave function) n (r)] E [n (r)].

[0102]That is, E [n (r)] is expressed by following formula (1201).

[0103]
[Equation 1]
Vz of the 1st paragraph of the right-hand side (r) assumes outer fields, such as a nuclear Coulomb field, the 2nd paragraph assumes the Coulomb interaction energy between electrons, and the 3rd paragraph assumes electronic one-body approximation, and it is the kinetic energy Ts [n (r)] in case there is no interaction between electrons, and is expressed by the following formula (1202).

[0104]
[Equation 2]
The 4th paragraph is the exchange correlation energy Exc [n (r)], and the form is based on partial density approximation. The electron density n (r) is expressed by the following formula (1203).

[0105]
[Equation 3]
A ground state solves the KS equation (Kohn-sham equation) showing in the following formula (21) and (22) which obtains the variations of E [n (r)] of an equation (1201) by setting it with 0, and it is used for it N pieces from the one where the characteristic value E is smaller. since n (r) is contained in the formula (1211) -- n (r), psi (r), and effective potential Veff (r) must be solved self-contradicting [no] (self-consistant).

[0106]
[Equation 4]
$[-**^2+V_{eff}$ (r)] psi(r) =Epsi (r) -- (1211)

$V_{eff}(r) =V_Z(r)+$integral -- 2n(r')/(|r-r'|) and dr'+deltaE$_{xc}$[n(r)]/deltan (r)

-- (1212)

The exchange correlation energy Exc [n (r)] obtained a following formula (1213) by applying and integrating partial density approximation (LDA) with the electron density n to energy epsilonxc per

electron (n).

[0107]

[Equation 5]

$E_{xc}[n(r)]$ =integralepsilon$_{xc}$(n (r)) n (r) dr —— (1213)

The form of epsilonxc (n) is proposed variously the formula besides Wigner etc. An inner shell electron is Vz of a formula (1211), when treating only a valence electron, without thinking. A nuclear Coulomb field is not used as it is as (r), but it sets by the norm preservation pseudopotential which erased the singularity in the nuclear position, and is a frog. The number of the ingredient in the Fourier expansion was able to be pressed down by accustoming in this way.

[0108]As total energy, this invention persons used the thing also containing the coulomb potential between atoms (ion) in order to expect ****. That is, it is a following formula (1221).

[Equation 6]

{R_I} is coordinates of the core of ion and {alphanu} is external constraints (volume omega, the strain epsilonLnu, etc.) here. The 1st paragraph of the right-hand side of a formula (1221) is Ts of the formula (1201) of DFT to the right-hand side. It is [n (r)] and the remainder of the formula (1201) right-hand side is one copy of U of a formula (1221). It is expressed with V_{eff} (r) from the formula (1211) of one-body approximation like the case of DFT, and the portion is Vz too. It uses by pseudopotential, replacing (r).

[0109]A new view was put in here. That is, it considers that E is potential energy and the virtual kinetic energy shown in a following formula (1222) is introduced into others.

[0110]

[Equation 7]

Therefore, a Lagrangian is expressed by the following formula (1223).

[0111]

L=K-E —— (1223)

Although M_I in a formula (1222) was the mass of the true atom (ion), mu and munu is virtual mass and was changed according to the purpose like the after-mentioned. The regular rectangular cross conditions shown in a following formula (1224) as a binding condition [Equation 8]

integralpsi$_i^*$(r, t) psi$_k$(r, t) dr=delta$_{ik}$ —— (1224)

Since it ****, a variations is taken, although undetermined-multipliers lambda$_{ik}$ was introduced and a following formula (1231) was added to L, when making the Eulerian equation. As a result, a following formula (1232), (1233), and (1234) are obtained.

[0112]

[Equation 9]

The temperature T of the kinetic energy of a formula (1222) corresponds. If it says by the relation of sigma1/2 $M_I R_I$2 because the degree of means has temperature each one by the energy equipartition law of classical statistical mechanics, it will be a temperature that it is not virtual and actual. psii and alphanu can be controlled or reinforced by the size of mu and munu.

[0113]For example, if it is referred to as T->0 from an elevated temperature as mu<<M_I, psii will change with R_I stopped and the ground state of an electron system will be acquired. The left side of an equation (1231) is set to 0 at this time, {lambda$_{ik}$} which makes the linear combination of psii suitably by the equation (1221) and the cautions under it since it becomes a following formula (30) is diagonal-lineized, and the right-hand side obtains a KS equation (1235).

[0114]

[Equation 10]

[**^{2}-V$_{eff}$ (r)] psi$_j$(r)+sigmapsi$_k$ (r) —— (1235)

That is, it means obtaining the same result as having solved the KS equation by DFT by simulated annealing. However, although the state of the temperature T is made, since it was not based on the Monte Carlo method but movement of the virtual dynamical system is followed, it is called dynamicalsimulated annealing (DSA).

[0115]When integrating with a formula (1231), psii cannot necessarily be treated as a variable as it is, but the expansion coefficient (that is, Fourier coefficient) which developed it by the plane wave can be treated as a variable. In order not to increase the number of this expansion coefficient recklessly, it is required like the case of DFT to erase the singularity in a nuclear position at pseudopotential. When the periodicity of a crystal can be used especially, the linear combination of psii which diagonal-line-izes above {lambda$_{ik}$} is described as phink. k is a wave number vector in a Brillouin zone, and n is a zone index.

[0116]phink should fill a following formula (1241).

[0117]

[Equation 11]

$$muS_{nk}(r, t) = [{**}^2 - V_{eff}(r)] \, phi_{nk}(r) + lambda_{nk} phi_{nk}(r, t) \quad -- (1241)$$

lambdank is a characteristic value of a procession {lambda$_{ik}$} and is an energy level. phink (r, t) is developed and a following formula (1242) is obtained.

[0118]

[Equation 12]

If pseudopotential is local (this condition generally is not fulfilled), effective potential V_{eff} will also be developed and a following formula (1243) will be obtained.

[0119]

[Equation 13]

A formula (1242) and a formula (1243) are substituted for a formula (1241), and a following formula (1251) is obtained.

[0120]

[Equation 14]

It is sigmaexp if it sets with K=K'+K'' in the time of the last of the right-hand side. Since [i(K+G) r] becomes common to all paragraphs, it removes, and a following formula (1252) is obtained.

[0121]

[Equation 15]

$$muT_{n, K+G}(t) = [-|K+G|^2 + lambda_{nk}] \, C_{n, \text{ and } K+G}(t) - sigmaV_{G-G}{}'(t) \, C_{n \text{ and } K+G}{}'(t) = -[|K+G|^2 + V_0(t) -$$

$$lambda_{nx}] \, C_{n \text{ and } K+G}(t). - sigmaV_{G-G}{}'(t) \, C_{n \text{ and } K+G}{}'(t) \quad -- (1252)$$

Frequency is defined here, as shown in a following formula (1253),[Equation 16]

$$omega = (|K+G|^2 + V_0(t) - lambda_{nx}) \, (/mu)^{1/2} \quad -- (1253)$$

If the left side of a formula (1251) is changed to difference, a following formula (1261) will be obtained.

[0122]

[Equation 17]

$$C_{n, K+G}(t + deltat) = 2cos(omegadeltat) \, C_{n, K+G}(t) - C_{n, K+G}(t - deltat)$$

$$-2 \quad -- [1 - cos(omegadeltat)] \, \{sigma_G{}'V_{G-G}{}'(t) \text{ and } C_{n, K+G}{}'(t)\}$$

$$-- (1261)$$

Since this formula is clearing up the integration of the vibrating part analytically, it can decrease computational complexity by making deltat larger than a numerical method purely.

[0123]The Coulomb potential is as follows. That is, this invention person found out being divided into the 4th paragraph, when the Coulomb potential was decomposed. Although there was only the 3rd paragraph in particular conventionally, it checked that there was the 4th paragraph newly. These methods are explained one by one.

[0124]This invention persons began to solve as a start of a strict formula first from the basic equation which considered the dielectric constant. It began to solve from the following formula (1262) which is a basic equation first.

[0125]

[Equation 18]

a conductor -- epsilon=infinity and in the case of the vacuum epsilon= 1, the Coulomb potential differs, L is taken by 1 ** of a unit crystal (cube), sigma is taken within a unit crystal, and Zi and ri are

electrifications and the positions of the i-th particle, respectively. This is because polarization arises in the inner surface of a ball by electrification in a ball. Although the layer of electric doublet is made in the inner surface of the ball which is not a conductor, the last paragraph of the above-mentioned formula serves to negate the effect exactly. Since the method of Ewald gives the thing of the left side and epsilon=infinity, it must add the last paragraph of the above-mentioned formula in quest of the value within a vacuum. Only a result is hung up.

[0126]A following formula (1271) shall express coulomb potential. [Equation 19]

In the formula (1271), the atomic number in a unit crystal, and atom [1st] position and electrification of N in it were ri and Zi, and n is a vector which specifies a unit crystal and the thing which shifted it periodically, and as shown in a following formula (1272), it was set up.

[0127]

$n = n_x Z_x + n_y Z_y + n_z Z_z$ -- (1272)

It is expressed. Zx, Zy, and Zz are the vectors of Tooru of x, y, and the direction of z here, respectively, and nx, ny, and nz are the integers ranging from -infinity to +infinity, respectively (in the case of a bulk crystal). It shall mean that ' of sigma' removes j=i at the time of n= 0.

[0128]This invention persons introduce here new F function shown in a following formula (1273).

[0129]

[Equation 20]

In the above-mentioned formula (1273), G (r, t) is a periodic function of t. This found out that it could express by Fourier series.

[0130]G (r, t) can change, as shown further below (1281).

[Equation 21]

In the above-mentioned formula (1281), m is a reciprocal lattice vector and is expressed by the following formula (1282).

[0131]

[Equation 22]

$m = m_x - (1/L_x, 0, 0) + m_y - (0, 1/L_y, 0) + m_z - (0, 0, 1/L_z)$ -- (1282)

The index mx, my, and mz are the integers ranging from -infinity to infinity, respectively. At the time of m= 0, it is exp. [--] Since it is =1, it is sigmaZi =0, and if the total electrification in a unit crystal is 0, a paragraph of m= 0 will disappear. If a paragraph of m= 0 is removed beforehand, it will become a following formula (1283).

[0132]

[Equation 23]

This invention persons divide an integral range by k, use two forms of G (r, t) properly, and get a following formula (1291).

[0133]

[Equation 24]

This invention persons used the following formula (1292) as formal here.

[0134]

[Equation 25]

Thereby, the Coulomb potential to begin is expressed by the following formula (1293).

[0135]

[Equation 26]

' seal at the upper right of sigma' means removing j=i at the time of n= 0.

[0136]A following formula (1301) is materialized.

[0137]

[Equation 27]

Since this formula (1301) does not contain r, it is not related to power. This formula (1301) can change, as further shown in a following formula (1302).

[0138]

[Equation 28]

When the above result is summarized, the Coulomb potential is expressed by following formula (1311) - (1315) after all.

[0139]
[Equation 29]
n is n=nx, +ny, and (0, Ly, 0) +nz− (0, 0, Lz) here, and m is m=mx, +my, and (1 [0 and]/Ly, 0) +mz − (1 [0, 0, and]/Lz). The point of the above-mentioned expression in good order is that decrease by the factor of erfc in phi (1), and the paragraph of sigma declines quickly by the factor of exp by phi (2) to the paragraph of sigma of a basis declining only to the order of a reciprocal in the paragraph of sigma. Since it is effective for reverse at slowness and fastness with attenuation by phi (3), it is necessary to choose suitable kappa which can balance both. These are the results of calculating contribution of Coulomb force sequentially from the near place of distance, and are results in case the circumference is moreover a conductor.

[0140]according to a case where the circumference is a vacuum −− already −− the 1st paragraph is added. Especially this is the portion which was not considered conventionally.

[0141]Generally in molecular dynamics, interatomic potential is the most important quantity. This also has fairly many that are simply described only in two bodies under the present circumstances. Time requires molecular dynamics calculation dramatically and a simple thing is being used for this for potential for the decrease of a clause of time. thus, if potential is made simple, the calculation itself will become quick, but it cannot be a thing reflecting the actual condition.

[0142]Generally important interatomic potential can be described to have described above by three bodies. The implications of this are as follows. Namely, it is effective in starting further first atomic (i) and an operation with the second atom (j) through the second (j) from the third atom (k). A thing illustrating this is drawing 4. Make r into distance between particles and let theta be a particle angle so that it may be shown in a figure. A relation of principal and accessory of these amounts of many is as being shown in drawing 5. It turns out that it is dramatically complicated so that it may understand especially by drawing 5. Although what differentiated potential generally becomes power, calculation becomes very complicated so that it may understand now. Here showed the position price of the conventional calculation technique and this invention once again using drawing 6.

[0143]This invention persons develop newly the Takashina round partial differential method in drawing 6, and enabled it to calculate it with high precision and at high speed by this. A actual comparative example is put into below and it is described in it how quick methods, such as this invention person, are. First, it cannot touch about simple potential calculation between two bodies in drawing 6 here. Because, since accuracy which almost bears for describing physical development of semiconductor LSI at use was not obtained, it decided not to argue here. On the other hand, this invention persons created a program of a table reference method as a conventional method by potential which put in a three-body problem. According to this, a table was created about r_{ij}, $theta_{ijk}$, and r_{jk}. Actually, as block data, arrangement was used and it stored. And a thing when it had shifted from this reference item was considered, and a complement program was also created. The cubic spline method was used for a complement. It was made a program which can quote a table about a certain value, i.e., r_{ij}, $theta_{ijk}$, and r_{jk}. However, desired conditions (r_{ij}, $theta_{ijk}$, and r_{jk}) need to explore into which procession within arrangement it goes. Although this invention persons created a program, distributing mind so that it may change as at high speed as possible, they needed a portion which divides too when based on a size of a number, and used an if then else sentence there. Thus, while finding out into which frame of a table desired conditions (r_{ij}, $theta_{ijk}$, and r_{jk}) fit, it is main ****** about a complement in it. Although potential in desired conditions (r_{ij}, $theta_{ijk}$, and r_{jk}) was able to be found now first, in fact, I want power in this point. In a portion which carried out the minute change, this invention persons searched for potential also about one more point using same procedure, and asked for differentiation, i.e., power, from both difference using an idea of an average rate of change.

[0144]Very many if then else procedure was used so that it might understand now. In an electronic computer, he is comparatively poor at if then else procedure, and it is slow. In fact, when a referred to type program which this invention person etc. created was used, it investigated for details only about a portion which calculates power. As a result, by a monocrystal substrate which consists of 1600 Si atoms, although it was a case with an external pressure of 1 atmosphere in the absolute temperature 300K, a referred to type program took about 350 times as much time. It turns out that the Takashina

round partial differential method which this invention person etc. propose is more advantageous so that it may understand now. In a referred to type program, whenever atoms differ, it is necessary to create a data table each time.

[0145]Next, a material property value etc. are extracted from molecular dynamics how, and it is also related for how putting it into a general-purpose simulator", and explains briefly.

[0146]Usually, evaluation art of all sorts is used in an LSI process. A property value appraisal method of a film by infrared absorption, stress evaluation in a film according to the Raman spectrum further, structural analysis of a film by X-rays, etc. occur. There is not only these optical things but electric evaluation art, such as a membranous dielectric constant.

[0147]It decomposed even into movement of an individual atom theoretically once wholeheartedly, and this invention persons pursued a principle of each evaluation technique in detail. Using molecular dynamics which this invention person etc. moreover developed, a motion of an individual atom was able to be pursued, and each evaluation quantity was able to be computed theoretically for the first time, for example, it was able to display directly on a form like a spectrum. Thereby, it is a reason for having obtained progress of big art which is not in the former that quantitive comparison with an actual measurement can be performed etc., for example.

[0148]this invention person etc. describe even pursuit of atomic movement by the first theoretical means to conquer, and derivation of the concrete amount of measurement evaluation below. Although there are some things, fundamentally, the fundamental concept which this invention person drew is as follows. That is, a moment of an atom to which its attention is paid is calculated. And this is integrated in a window of time to pay one's attention, the Fourier transform is carried out to after an appropriate time, and an inherent spectrum is obtained. This is a big main point.

[0149]Next, Si is shown [experiential] for how this invention person changed the potential into power by being related potentially in an example. Although this is an example, if it does not take into consideration an effect not only by Si but an ionic bond, the Takashina round partial differential described here can be used for it as a three-body problem, for example like [potential of an oxide film] a problem of this Si. What kind of potential is good examined this invention persons about Si.

[0150]Potential used here is based on Tersoff. (Phys.Rev.Lett.56.632 (1986), Phys.Rev.B37-6991 (1988)).

[0151]Total potential [according to now and Tersoff] about i-th Si, [Equation 30]

It can come out and describe. Since three bodies have described this, it is $V_{ij} \neq V_{ji}$ in the above-mentioned formula (0001) that this invention person etc. want to call attention. When the location number of Si atom to which its attention is paid is set to i and other particle numbers of the circumference of it are set to j, the above-mentioned V_{ij} is,[Equation 31]

$$V_{ij} = f_c (r_{ij}) [a_{ij} f_R(r_{ij}) + b_{ij} f_A (r_{ij})] \ \text{---} \ (0002)$$

It comes out. r is the distance between particles here. $f_c (r_{ij})$ is a cutoff function, $f_R (r_{ij})$ shows repulsive force and $f_A (r_{ij})$ shows attraction. a_{ij} are a cutoff coefficient in consideration of the coordination number, and the cutoff coefficient as which b_{ij} also considered the coordination number. Three-body expression will be performed using a parameter expressing the coordination number. Since a basic form is the same in other things, this shows below here, mixing thought of the first round technique for this invention person etc. to develop.

[0152]$f_R (r_{ij})$ and $f_A (r_{ij})$ are what changed Morse type potential, and are $f_R(r_{ij}) = A\exp(-\text{lambda1} r)$ and $f_A(r_{ij}) = -B\exp(-\text{lambda2} r)$.

[0153]Among this, lambda1 and lambda2 are constants, and that size is a reciprocal of a value about interatomic distance.

[0154]By the way, the cutoff function $f_c (r_{ij})$, [Equation 32]

$$V_{ij} = f_c (r_{ij}) [a_{ij} A\exp(-\text{lambda}_1 r_{ij}) - b_{ij} B\exp(-\text{lambda}_2 r_{ij})]$$

$$f_c (r) = 1 \ (r \leq R-D)$$

$$f_c(r) = 1/2 - 1/2 \sin [\text{pi}/2(r-R)/D] \ (R-D < r < R+D)$$

$$f_c (r) = 0 \ (r \geq R+D)$$

-- (0003)
It comes out, and it is, and R chooses the size here so that only the first adjacent zone of the target structure may usually be included. According to this invention person's detailed examination, the value is about 2-3A. Next, although b_{ij} will show the real coordination number, it uses the above-mentioned

cutoff function also here. According to Tersoff, the definition is $b_{ij}=(1+beta^n zeta_{ij}^n)^{-1/2n}$. -- (0004)

It comes out. Here, [Equation 33]

$zeta_{ij}=sigma f_c(r_{ik}) g(theta_{ijk}) exp[lambda_3^3(r_{ij}-r_{ik})^3]$ -- (0005)

It comes out. sigma sign turns by k!=i and j. Since the meaning of $zeta_{ij}$ is an environmental factor by the 3rd atom k entering as it understands here, it is with the case where it sees from i, and the case where it sees from j, and sizes differ mutually. That is, it is $zeta_{ij}!=zeta jij$, and further, as the above-mentioned formula (0001) described, it is $V_{ij}!=Vji$. Therefore, it is $b_{ij}!=bji$.

[0155]g (theta) is a bond angle factor, [Equation 34]

$g(theta)=1-(c^2/d^2)-c^2/(d^2+costheta^2)$ -- (0006)

It comes out. Here, theta shall be taken like drawing 4. In asking for theta, it expresses using actual rectangular coordinates. namely[Equation 35]

$r_{ij}=root\{(x_j-x_i)^2+(y_j-y_i)^2+(z_j-z_i)^2\}$ -- (0007)

It comes out, and it is and r_{ik} is also called for in same procedure. If it does so and an inner product will be made into P_{ij},[Equation 36]

$P_{ijk}=(x_j-x_i)(x_k-x_i)+(y_j-y_i)(y_k-y_i)+(z_j-z_i)(z_k-z_i)$ -- (0008)

It comes out. These are used and it is $costheta_{ijk}=P_{ijk}/(r_{ij}-r_{ik})$. -- (0009)

It becomes. Here, the constant in each above-mentioned formula which this invention person etc. used is shown. namely[Equation 37]

R= 3.0 A, D= 0.2 A, A=3264.7ev, B=95.373ev, C= 4.8381, $lambda_1$=3.2394A, $lambda_2$=1.3258A, $lambda_3$=$lambda_2$, beta= 0.33675, n= 22.956, and d= 2.0417 -- (0010)

It comes out.

[0156]this invention person's round portion is explained in detail still more through these preparations. From here, power is calculated still more and it goes. It will become power if a potential (0002) formula is differentiated from coordinates of a position. namely[Equation 38]

It is x ingredient of the vector of power which works to ********* and the particles i and j. However, it is not so easy to actually ask for it. Below has the device and invention which stood on this invention person's etc. mathematical theories, and returned. It is the division called Takashina round partial differential.

[0157](0011) What is necessary is just to carry out partial differential of the formula described by the formula and (0012) the formula concretely. However, it turns out immediately that it is not so simple.

[0158]namely[Equation 39]

Modification of the partial differential equation about j and k is as follows similarly. Although the above mainly described x, it is necessary to perform it also about y or z. A blank part keeps blank and was placed especially here so that correspondence with the above might be known. Such complicated modification was not found as long as this invention person etc. investigated. Such complicated modification was conquered until now and, for the method reason of ****, it had escaped to the simple table reference method conversely. Since such an invention was conquered, this invention persons have united molecular dynamics and a general-purpose fluid simulator.

[0159]

[Equation 40]

Each item of these formulas can change as follows.

[0160]

[Equation 41]

$**V_{ij}/**r_{ij}=**f_c(r_{ij})/**r_{ij}$ and $[Aexp(-lambda_1/r_{ij})-b_{ij}Bexp(-lambda_2/r_{ij})]+f_c(r_{ij})[-lambda_1Aexp(-$

lambda$_1$/r$_{ij}$)+lambda$_2$b$_{ij}$Bexp (−lambda$_2$/r$_{ij}$)]

= Aexp. (−lambda$_1$/r$_{ij}$) −[**f$_c$(r$_{ij}$)/**r$_{ij}$−lambda$_2$f$_c$(r$_{ij}$)]− Bexp(−lambda$_2$/r$_{ij}$) − [**f$_c$(r$_{ij}$)/**r$_{ij}$−lambda$_2$f$_c$ (r$_{ij}$)] b$_{ij}$ −− (0016)

f$_c$(r$_{ij}$)/r$_{ij}$=−pi/4 D−cos[pi/2−(r−R)/D]

(R−D<r<R+D)

f$_c$(r$_{ij}$)/r$_{ij}$=0 (r>=R+D)

−− (0017)

V$_{ij}$/zeta$_{ij}$=. (**V$_{ij}$/**b$_{ij}$) −. (**b$_{ij}$/**zeta$_{ij}$). = −Bfc. (r$_{ij}$) exp−. (lambda2r$_{ij}$) −$^{1/2n-1}$beta^{n}zeta$_{ij}$$^{n-1}$=Bfc (r$_{ij}$) exp−(lambda2r$_{ij}$) b$_{ij}$(betazeta$_{ij}$) ^{n}/(−1/2n) (1+beta^{n}zeta$_{ij}$^{n}) [2{1+(betazeta$_{ij}$) ^{n}} zeta$_{ij}$]

−− (0018)

zeta$_{ij}$/r$_{ij}$=3lambda$_3$^{3}sigmaf$_c$(r$_{ik}$) g(theta$_{ijk}$) exp(lambda$_3$^{3}(r$_{ij}$−r$_{ik}$) ^{3}) (r$_{ij}$−r$_{ik}$) ^{2} −− (0019)

[Equation 42]

zeta$_{ij}$/r$_{ik}$=df$_c$. (r$_{ij}$)/dr$_{ij}$ and g(theta$_{ijk}$) exp (lambda$_3$^{3}(r$_{ij}$−r$_{ik}$) ^{3})−3lambda$_3$ ^{3}f$_c$(r$_{ik}$) f$_c$(r$_{ij}$) (r$_{ij}$−r$_{ik}$) ^{2} −− (0020)

zeta$_{ij}$/costheta$_{ijk}$=f$_c$. (r$_{ik}$) exp. (lambda$_3$ ^{3}.) (r$_{ij}$−r$_{ik}$) ^{3}dg (theta$_{ijk}$/dcostheta$_{ijk}$f$_c$(r$_{ik}$) exp(lambda$_3$^{3}(r$_{ij}$−r$_{ik}$) ^{3}) [2c^{2}costheta$_{ijk}$/{d^{2}cos^{2}theta$_{ijk}$} ^{2}].) −− (0021)

r$_{ij}$/x$_i$=(x$_i$−x$_j$)/r$_{ij}$=**r$_{ij}$/**x$_i$ −− (0022)

r$_{ik}$/x$_i$=(x$_i$−x$_k$)/r$_{ik}$=**r$_{ij}$/**x$_k$ −− (0023)

[Equation 43]

** −− cos −− theta −− $_{ijk}$ −− −− /−− ** −− x −− $_i$ −− −− = −− one −− /(r$_{ij}$r$_{ik}$) − ** −− P −− $_{ijk}$ −− −− /−− ** −− x −− $_i$ −− $^{- + -}$ −− P −− $_{ijk}$ −− −− {−− one −− /(r$_{ik}$) −− ** −− /−− ** −− x −− $_i$ −− −− [−− one −− /(r$_{ik}$) −−] −− $^{- + -}$ −− one −− /(r$_{ij}$) −− ** −− /−− ** −− x −− $_i$ −− −− [−− one −− /(r$_{ik}$) −−] −−}

= 1/(r$_{ij}$r$_{ik}$) −(x$_i$−x$_k$+x$_i$−x$_j$)− P$_{ijk}${(x$_i$x$_j$)/(r$_{ik}$r$_{ij}$^{3})+(x$_i$−x$_k$)/(r$_{ik}$r$_{ij}$^{3}). = 1/(r$_{ik}$) −{(x$_i$−x$_j$) /(r$_{ij}$)− /(x$_i$−x$_k$) (r$_{ik}$) costheta$_{ij}$}

−− (0024)

costheta$_{ijk}$/x$_i$=−1/(r$_{ij}$) and {(x$_i$−x$_k$)/(r$_{ik}$) −(x$_i$−x$_j$)/(r$_{ik}$) costheta$_{ij}$} −− (0025)

costheta$_{ijk}$/x$_k$=−1/(r$_{ik}$) and {(x$_i$−x$_j$)/(r$_{ij}$) −(x$_i$−x$_k$)/(r$_{ik}$) costheta$_{ij}$} −− (0026)

L (r$_i$**r$_i$/**t, V, **V/**t) =1/2sigmam(**r$_i$/**t) ^{2}−U(r$_i$)+1/2M(**V/**t)^2−P$_E$V−(**L(q$_j$, q'$_j$)/**q$_j$) d (**L/**q'$_j$)/dt=0 −− (0027)

Cooperation with the above−mentioned process variation calculation unit I is explained to drawing 7 and drawing 8 as the molecular dynamics simulator II. There are some which are transmitted as the first input a from a file (22) shown in drawing 8, (32), (42), (52), (62), (72), etc. in the molecular dynamics simulator II. the contents −− a boundary condition, and area size (namely, breadth of a x direction, breadth of a y direction, breadth of the direction of z) and stress (namely, sigmax, sigmay, sigmaz) −− it is distorted (namely, epsilonx, epsilony, epsilonz) and is temperature etc. There is the input b auxiliary as the second thing if needed, and there are computation time of molecular dynamics, specification of ensemble, etc.

[0161]On the other hand, position vector r (t) comes out as the first output. And it is transmitted to a file (23) shown in drawing 8, (33), (43), (53), (63), (73), (83), etc. Membrane characteristics, such as optical, electric, and crystallographic characterization, are computed, and it is transmitted to a file (3) of drawing 8 by ** and the membrane−characteristics calculation program III.

[0162]An example of an input sequence of wide use 2 and a three−dimensional process simulator ((Ia) of drawing 8) is shown in drawing 9. wide use 2 and a three−dimensional process simulator ((10) of drawing 8) will accept it as well as drawing 10 −− one input sequence is shown. While contents shown in drawing 9 also specify a cluster tool used, respectively, for example, there are gas volume, a temperature−up sequence, a valve sequence, etc. in details of an oxidation process which is, for example in it.

[0163]On the other hand, an input sequence of drawing 10 is a case where strange material shown by drawing 8 is included. In the case of this drawing 10, it is a ferroelectrics film, and it includes a process of carrying out the weld slag of the film, for example. Since there is no detailed data of a ferroelectrics film at this time, it flies to the molecular dynamics simulator II, and is once calculated there at it.

[0164]This invention persons perform a molecular dynamics simulation which gave experiential potential, (1) A superposition phenomenon of fluctuation of each process element or a gap of each element was also diagnosed, and a simulation system which also enables a check of whether to perform as a sequence of (2) requests and discovery of (3) change factors was developed.

[0165]While proposing physical relationship of a single crystal ferroelectrics film and a Si substrate, and position relation with a metal electrode, specifically, an indicator was able to be further shown for the first time also about what quality of a thing should be prepared in practice as a single crystal ferroelectrics film. While reproducing this single crystal ferroelectric membrane structure with the original calculation technique using a computer strictly, a characterization function is given, ****** and impression conditions are considered to this, and what should be done with physical relationship with a substrate single crystal to it, or [simultaneously] an indicator of tolerance level of the defect density is shown.

[0166]This invention persons invented a method of carrying out calculation prediction of various phenomena in a system which contains an element variously at high speed and with high precision by a new computational chemistry theory. By this, the characteristic of various materials used for a semiconductor manufacturing process can calculate now with high precision.

[0167]As a means to predict conventionally structure and the characteristic of a crystal or a molecule that an element is contained variously, an abinitio molecular dynamics method and a ultimate cause molecular orbital method have been used. An abinitio molecular dynamics method was mainly used for structure of a crystal, or investigation of an electronic state, and a molecular orbital method has been used for performing calculation of the structure and electronic state for a cluster which cut down the usual molecule and some crystals. However, in these methods, in order to solve a Schrodinger equation to each electron of a system, huge computation time was required. Therefore, it was actually impossible to have incorporated these ultimate cause technique in the technique of needing calculation times of several 100,000 steps like a molecular dynamics method which gave experiential potential. On the other hand in the field of molecular dynamics, A.KRappe and W.A.Goddard in a paper of "Charge Equillibration for Molecular Dynamics Simulations" in 1991, The new electric charge calculation technique for a polyatomic molecule is proposed. This invention persons extend still more greatly the electric charge calculation technique in a polyatomic molecule proposed by A.R.Rappe and others, It changed substantially so that it could apply to various elements and crystal systems, and a materials design simulation procedure applicable also to PbTiO3, a ferroelectric called PZT, and a high dielectric was built as well as Si and SiO_2 which are generally used as a material of a semiconductor device. First, the technique of Rappe and others is described below.

[0168]Rappe and others considered the energy E of an isolated atom as a function of ionization potential and electron affinity first. That is, in a certain atom A, A0 shows a neutrality state electrically. If it thinks to the secondary paragraph of Taylor's expansion, [Equation 44]
An atom is obtained by the energy of a neutrality state substituting zero for QA of a formula (3031) electrically.

[0169]
$$E_A (0) = E_{A0} \quad -- (3041)$$
When an atom +−1−value−ionizes, energy is acquired by substituting one for QA of (3031), and when it ionizes to −1 value, energy is acquired by substituting −1.

[0170]
[Equation 45]
The difference of (3042) and (3041) is set to ionization potential IP, and the difference of (3043) and (3041) becomes the electron affinity EA.

[0171]
[Equation 46]
(3045) When it considers it to be positive work to take an electron, − is attached to EA of a formula in

order to mean that adding an electron had done negative work. If the difference of (3044) and (3045) is taken, it will become the electronegativity chiA0.

[0172]
[Equation 47]
A following formula will be realized if the sum of (3044) and (3045) is taken.

[0173]
[Equation 48]
Here, the physical meaning of a formula (3052) is considered. The mimetic diagram of the Coulomb interaction at the time of the ionization in the case of a hydrogen atom is shown in drawing 12 thru/or drawing 14. As shown in a figure, the difference of IP and EA is Coulomb interaction between electrons b. Therefore, it is IP−EA=J_{AA}^{0} when the coulomb repulsive force between 2 electrons in phiA orbit is expressed as JAA0. −− (3053)
JAA0 will be called idempotential. Since orbital shape changes by adding an electron, some values of JAA calculated by ultimate cause calculation of Hartree−Fock etc. and a formula (3053) differ, but it approximates by a formula here (3053).

[0174]The relation between Idempotential JAA0 and atomic diameter RA0 is considered. Considering the easy atomic structure model shown in drawing 15, Coulomb interaction JAA0 between electrons is as follows.

[0175]
[Equation 49]
Here, JAA0 is eV unit and R is ** unit. (3053) In order to check the validity of a formula, the relation between J value and R was investigated and it collected into Table 1. As shown in Table 1, J was mostly inversely proportional to atomic sizes, and it turned out that the diameter of the atom called for from the formula (3054) is about in agreement with homopolar bond distance.

[0176](3051) If a formula is used, energy (3031) of an isolated atom can be written with a following formula (3053).

[0177]
[Equation 50]
In the case of a polyatomic molecule, it is necessary to also take the electrostatic energy between atoms into consideration. Electrostatic energy can be expressed with a following formula.

[0178]
[Equation 51]
Here, JAB is a Coulomb interaction in case there is 1 electron charge at the center of the atoms A and B. JAB is dependent on the distance between AB(s). (3055) When a formula is used, all the electrostatic energies can be expressed with a formula (3057).

[0179]
[Equation 52]
Chemical potential chiI (Q1, …, QN) of an atomic scale can be expressed with a following formula.

[0180]
[Equation 53]
The simultaneous equations of KA (N−1) are obtained from the conditions (3059) of an electric charge balance.

[0181]
$chi_1=chi_2=$ …… $=chi_N$ −− (3059)
namely [Equation 54]
It becomes. To this, N simultaneous equations including the condition (3062) equation of all the electric charges are solved.

[0182]
[Equation 55]
(3061) When it displays by a matrix, it can express with the following formulas (3062).

[0183]
[Equation 56]
(3063) Since a maximum minimum is among the electric charges which each ion can take in solving a

formula, if an electric charge becomes in the range outside, fix the electric charge to a boundary value. (3061) It separates into the electric charge which fixed the formula to the boundary value, and the electric charge which is not so, correct a formula (3063), dispel a matrix, and make it converge. Then, dispersion in an electric charge is calculable.

[0184]All that matters in this method is the determination of JAB. When the distance RAB with the atoms A and B is large [Equation 57]

Although it is easy to come out, it is necessary to consider repulsive force in distance with which an electron cloud laps. Here, electron density will be approximated by a paragraph of the one Slater orbital. That is, in ns, np, or an atom that is nd, an outside valence orbital presupposes that it consists of the ns Slater orbital by which the following mold was standardized in any case.

[0185]

[Equation 58]

(3065) If it asks for atomic average size using a formula,[Equation 59]

It becomes. Valence orbital index zetaA is chosen with the following relation.

[0186]

[Equation 60]

lambda is a parameter for adjustment, and it is contained in order to calculate the difference of the average atomic sizes and covalent-radius RA of a crystal which were given by the formula (3066).

[0187]The scaling parameter lambda is set up using an alkaline metal halide molecule as shown in drawing 16. An alkaline metal halide molecule is set to MX, and use M as an alkaline metal (Na, K, Rb, Cs), and let X be halide (Cl, Br, I). When each electric charge is expressed as QM and QX, it is $Q_{total}=Q_M+Q_X=0$ therefore$Q_X=-Q_M$ from a formula (3062). -- (3068)

(3061) From a formula [Equation 61]

(3069) If a formula (3068) is substituted for a formula,[Equation 62]

$(J_{MM}-J_{MX}-J_{XM}+J_{XX}) Q_M=chi^0{}_x-chi^0{}_M$ -- (3071)

By the way, it is $J_{MX}=J_{XM}$ clearly. -- (3072)

Because it comes out, [Equation 63]

(3073) The variable of a formula is only lambda. Dipole moment muMX is calculated using a formula from calculated Q (3074), and lambda is determined as compared with an experimental value.

[0188]

$mu_{MX}=4.80324Q_M R_{MX}$ -- (3074)

RMX is an experimental value of bond distance. (3074) As for the formula, Q becomes, R becomes ** per e, and mu has become a unit of a debye. 0.4913 is obtained from comparison with the experimental value of a dipole moment as an optimum value of lambda. If this lambda is used (3067), the valence orbital index zeta can be found in the value of the table of drawing 17 from a formula.

[0189]About hydrogen, Rappe and others is doing different handling from other elements.

[0190]As compared with Mulliken and a value on an experiment of Pauling others, it is not in agreement in electronegativity of hydrogen. On a Mulliken scale, hydrogen is electronegativity from carbon or nitrogen to hydrogen being electropositivity from carbon and being electronegativity in a Pauling scale, more slightly than boron. Since the orbit of hydrogen which has combined a problem of this electronegativity cannot spread like a free hydrogen ion, it is because it becomes smaller than a value in case the execution electron affinity EA is an atom.

[0191]Therefore, EAH is made into a variable and chi0H of hydrogen and J0HH are redefined.

[0192]

[Equation 64]

It is $chi^0{}_H=4.528eV$ $J^0{}_{HH}(0) =13.8904eV$ by comparison with an experiment to the least square method. -- (3076)

Not an experiment but the comparison with the electric charge calculated from the electrostatic potential of HF wave function to $chi^0{}_H=4.7174eV$ $J^0{}_{HH}(0) =13.4725eV$ -- (3077)

It is supposed that it may be used.

[0193]A boundary value about an electric charge is set up.

[0194]A valence shell is not appropriate to chi_A^0 and J_{AA}^0 out of a range corresponding empty or to the limit clearly. For example, in Li, C, and O, an electric charge is restricted at a range as shown in the following figure. $E_A(Q)$ =infinity is taken out of this range.

[0195]It judges whether it is within the limits of inequality showing an electric charge which dispelled and searched for a matrix (3063) in drawing 18 thru/or drawing 20, and in being outside the range, it fixes the electric charge to a boundary value.

[0196]The above is an outline of the technique of Rappe and others. Rappe and others has applied the above-mentioned technique to a molecule of an organic system. This invention persons adopted only a concept of chemical potential of an atomic scale which Rappe and others proposed, and newly developed the individual atomic charge calculation technique in a crystal system. The electric charge calculation technique by this invention persons is described below.

[0197](3057) The second paragraph of the formula right-hand side means the sum of electrostatic energy of all the combination. This invention persons extended to a crystal from a molecule, and tried a periodic boundary condition with a method of introduction. Then, when calculating electrostatic energy, it discovered that it was necessary to take into consideration not only hundreds - thousands of atoms that are used for calculation but electrostatic energy received from a countless virtual atom on the outside. That is, attenuation of electrostatic energy was small and he has noticed that influence from a distant atom is also steamed and is not made. Then, electrostatic energy from a virtual cell was also taken into consideration, assuming that a countless cell exists in the outside of a cell used for calculation virtually.

[0198]In this case, as for the electrostatic energy JAB received from an atom in a formula (3057) virtual cell, when a size of and calculation cells is taken into consideration, RAB is usually a big value of 10 A or more. Since it becomes, Coulomb energy and ** may obtain. Therefore, JAB=1/RAB, and 1 It treats to **. If a virtual cell is expressed with nu, a formula (3051) will be changed as follows.

[0199]
[Equation 65]
Here, nu= 0 means the calculation cells themselves and nu!=0 means a virtual cell. (3078) Apply the Ewald method to the 3rd paragraph of a formula. If the Ewald method is used, the 3rd paragraph can be searched for as follows.

[0200]
[Equation 66]
It is a parameter in which G adjusts a reciprocal lattice vector, omega adjusts the volume of calculation cells, and kappa adjusts convergence of the Ewald calculation. The first paragraph of the formula (3082) right-hand side does not include the paragraph of nu= 0 and A=B, and the second paragraph does not include the paragraph of G= 0. If it asks for chemical potential chiI of an atomic scale from these formulas,
[Equation 67]
It becomes. N-1 equation is obtained from conditions of an electric charge balance.

[0201]
$chi_1=chi_2=chi_3= .... =chi_N$ -- (3092)

(3091) Substitute a formula, [Equation 68]
(3093) N simultaneous equations which can be expressed with an equation will be solved.

[0202](3093) A following formula will be obtained if the matrix of CQ=-D is made from a formula.

[0203]
[Equation 69]
This invention persons discovered that what is necessary was just to solve a formula, taking a periodic boundary condition into consideration, when the crystal and amorphous substance like SiO_2 were treated (3094). (3094) To the electric charge Q, since a formula is nonlinear, it brings the loop for completing Q to a calculation program.

[0204]This invention persons also paid attention to modeling of the Coulomb integral which is in charge of real calculation. JAB was calculated as a two-atom Coulomb integral of the Slater function over zetaA and zetaB. Coulomb integral JAB. It calculated using the method of ** Roothern. Roothern and others uses the sign of being in Coulomb integral JAB. (3101) A Coulomb integral can be expressed with a

formula (3102) using the parameter defined by the formula.
[0205]
[Equation 70]
Here[Equation 71]
(alpha, alpha', beta, beta')
$= (1+tau_a)$ alpha$(1-tau_a)$ alpha'$(1+tau_b)$ beta$(1-tau_b)$ beta' -- (3103)
It comes out. Further,[Equation 72]
Here, the unit systems of an upper type are atomic units, distance uses bohr and energy is using Hartree.
[0206]Although Roothern and others had given the analysis formula of the Coulomb integral to 1s, 2s, and 2p, this invention persons calculated to the Coulomb integral over the atomic orbital after 3s, and they chose the optimal orbit so that Si and SiO_2 which are generally used with a semiconductor device could be treated.
[0207]The value of JAB influences electric charge calculation greatly. Therefore, setting out of the Slater orbital used when computing J, or the valence orbital index zeta is important. Then, this invention persons investigated about the value of J in the case of treating Si-O and Si-Si.
[0208]Although it is carrying out "assuming if polarization charge is in ns orbit" Rappe and others, a point whether it is optimal taking which orbit into consideration to an element variously is unknown. Since the principal quantum number n of Si was 3, it compared by performing calculation a case where a model is made when an electric charge of Si was in 3 s, and at the time of assuming that it is in 2 s. At this time, this invention persons prepared an analysis type of J in n= 3 separately in accordance with a method of Roothern. For example, a following formula was used to Si-Si.
[0209]
[Equation 73]
Drawing 21 is a calculation result of Coulomb interaction J between Si-Si. In this case, even if it uses any (2s and 3s), it turns out that there is almost no change in the value of J. However, Coulomb interaction J between Si-O differs greatly by the case where 2s and 3s are used. The electric charge of O is shown in drawing 22 at 2 s, and the calculation result of JAB at the time of making a model, when Si was in 2 s or 3 s was shown. In response to the influence to which 3 s orbits have spread dramatically, the value of J will have [in / for the electric charge of Si / 3 s] the minimal value at nearly r= 1.6A. Since the bond distance of Si-O was in this hit exactly, J estimated very small and it turned out that a result and any electric charge of Si and O will be evaluated too little [very]. The same might be said of the case of Si-H. Therefore, as a model of the electric charge of Si, if it dares to assume by 3 s orbits, the estimate of J will completely lack accuracy. From this, it was only in order to take the breadth of an electric charge into consideration to use the Slater orbital, and it was understood that it is optimal as a model to use the Slater orbital for 1 s or 2 s. This was the same also to the element of the atomic number after Si, and when the orbit it spread after [whose] 3s was used as the model, it turned out that the calculation precision of Coulomb force when interatomic distance is near gets very bad.
[0210]This invention persons also paid attention on a program to amendment to hydrogen. (3031) From a formula, [Equation 74]
Chemical potential chiHI of an atomic scale when hydrogen amendment is carried out is calculated. First, the formula of the energy of the polyatomic molecule corresponding to a formula (3057) is, when it is M hydrogen among all the N atomic numbers, [Equation 75]
Here, when the sign of sigma' of the first paragraph of the right-hand side of a formula (3114), the second paragraph, and the fifth paragraph asks for each sum, it means that H is removing. Chemical potential chiHI of an atomic scale, [Equation 76]
(3121) The fourth paragraph of the formula right-hand side can be unraveled as follows.
[0211]
[Equation 77]
(3122) A formula shows that the sum of the fourth paragraph of (27) types and the fifth paragraph means the Coulomb interaction between atoms between all the atoms other than HI. Therefore, chemical potential, [Equation 78]

(3123) Change will be added to a matrix (3063) at the time of hydrogen amendment using a formula. Now, a formula (3123) will be substituted for a formula (3059) supposing chi 1 is atoms other than hydrogen, [Equation 79]

As compared with a matrix (3063), it is about JiiO of hydrogen.[Equation 80]

It is alike and will change.

[0212]Next, hydrogen amendment of the Coulomb potential JAH between atoms is considered. The Slater orbital function in the case of hydrogen is a formula (3075), [Equation 81]

When hydrogen is contained, after searching for an electric charge, a formula (3126) is used, JAH is corrected, and an electric charge is searched for again. And this is repeated until it is completed by the value of an electric charge. Under the present circumstances, when the line of I= 1 was hydrogen, this invention persons created the algorithm so that it might change for the line which is not hydrogen and a matrix might be created.

[0213]This invention persons also paid attention to the treatment of an electric charge boundary condition for the concrete changing method of the matrix.

[0214](3061) Divide a formula into electric charge QC which is not so, and consider it to be the electric charge QB fixed to a boundary value.

[0215]

[Equation 82]

(3062) When a formula is changed into a formula (3131), the element of a matrix is at the ** time, [Equation 83]

A matrix is changed like an upper type and an electric charge is stored within the limits of a boundary condition. When the element of I= 1 was set as a boundary value at this time, it was made to choose the line so that the line of a matrix might be replaced and the line to the element by which boundary-value setting out is not carried out might be set to I= 1 (pivoting).

[0216]They computed the IR spectrum by this invention persons having added this to the molecular dynamics method, having calculated the motion of an individual atom one by one using the above-mentioned electric charge numerical orientation method newly developed in the crystal system and the amorphous system, having calculated the dipole moment every moment, having recorded it, and having done the Fourier transform of this. Drawing 23 summarizes the above procedure.

[0217]On the other hand, in the gate oxide used for DRAM after 16G, or the tunnel oxide film of NAND EEPROM, high reliability-ization has been important SUBJECT also compared with the former. In order to use an oxide film under the severe condition of maintaining insulation, in EEPROM especially, sending tunnel current under a high electric field, it is important to search an atom and an electronic level for the limit as an insulating material.

[0218]From such a situation, a search experiment with an atom level of Si/SiO_2 interface structure or SiO_2 network structure, an experiment of a trap mechanism of SiO_2, prediction by theoretical calculation, etc. are advanced in various research institutions. However, like this invention, relation of network structure and IR full spectrum was associated with an atom level, and there was no technique to be used in the former. an experimental result which associates an asymmetric stretch peak of Si-O of an IR spectrum, and stress of an oxidation interface slightly -- a report -- now, it was only.

[0219]Only an argument from a vibration analysis of Si-O-Si molecular structure which simplified an actual network dramatically is made using a "central force model" also as an interpretation of an experimental result, It did not have a discussion in consideration of all distribution of distribution of amorphous characteristic Si-O bond length, Si-O-Si, and the degree of O-Si-O bond angle at all conventionally. In this invention, correlation with an electrical property and structure was acquired from a different viewpoint from a central force model by taking into consideration these amorphous characteristic various distribution.

[0220]Here, it adds about a point which this invention persons conquered. In using a classic molecular dynamics method, this invention persons examined the potential, and also they added improvement further. Although this invention persons tried use of TTAM potential developed by Mr. **** and others at first, they found out a fault that Si-O asymmetric stretching vibration was dramatically expressed to the low wave number side. Then, BSK potential developed by van Beest etc. was used. As for their potential, an elastic peak was expressed with a wave number lower in addition than an actual

measurement although a peak appeared in the number side of Takanami also in a TTAM potential twist.

[0221]In order that this invention persons might bring this peak value close to survey, they removed conditions of electric charge regularity currently used by these existing potential, and incorporated distribution of an electric charge when a Si-O-Si angle etc. are situated very much into classic molecular dynamics. Calculation of dealing with hundreds of atoms structure at once, and performing electric charge distribution calculation as an actual problem, under the present circumstances although calculation of this electric charge distribution is ideally computable using a molecular orbital method It is actually impossible even if it uses a supercomputer.

[0222]Then, this invention persons performed electric charge distribution calculation using a technique proposed by A.R.Rappe and W.A.Goddard III. Citation papers are "Charge Equillibration for Molecular Dynamics Simulation", J.Phys.Chem., 95 and 1991, and p.3358-3363. This invention persons developed expression for their paper to reference, after correcting an error in a paper, they performed required parameter calculation uniquely, and they applied the technique of them to a SiO_2 system. An outline of the technique of Rappe and others is described below.

[0223]Energy Ei by an individual electric charge of the atom i (Q) is considered to the 2nd order of Taylor's expansion, and is approximated with a following formula (1651).

[0224]
[Equation 84]

Here, Xi 0 is electronegativity and it is expressed with a following formula (1652).

[0225]

$X_i^0 = 1/2 \ (IP + EA) \ -- \ (1652)$

Jii is the coulomb repulsive force between the electrons on the orbit of the atom I, and is defined by the following formula (1661).

[0226]
Jii=IP-EA -- (1661)

As for IP, ionization potential and EA show an electroaffinity here. Total energy E (Q1, --, QN) of the molecule which comprises N atoms is the energy of an individual atom, and the sum of interaction electrostatic energy J_{ij}Qi Qj between atoms. However, J_{ij} is a Coulomb interaction of the unit charge which exists at the center of atomic $_{ij}$. Therefore, a following formula (1662) is materialized.

[0227]
[Equation 85]

The chemical potential of an atomic scale is given with a following formula (1663).

[0228]
[Equation 86]

The conditions of the electric charge balance by this formula (1663), X1 = -- If it substitutes for =XN, a following formula (1671) will be obtained.

[0229]
[Equation 87]

That is, a following formula (1672) is obtained.

[0230]
[Equation 88]

The conditions of all the electric charges shown in a following formula (1673) are taken into consideration.

[0231]
[Equation 89]

J_{ij} is known and is a following formula (1674) about.

[0232]
[Equation 90]

R is interatomic distance here at the time of an atomic size and I!=j at the time of I=j. Therefore, introduction of the procession C and the vector d will form the simultaneous equations showing in the following formula (1681) about Q. namely[Equation 91]

It is CQ=-d if a definition is given. -- (1682)

It becomes. Although it was with C1 i=Qi and Cd =d in the paper, this invention persons used these, having corrected them as mentioned above. Required parameters, such as a size of atoms, such as Si-O-H, were computed uniquely, simultaneous equations were solved, and electric charge distribution was searched for. by this, a peak wave number is markedly alike and in agreement with survey. [came]

[0233]An example of "a family register computed by the molecular dynamics simulator II", i.e., a vast quantity of data in which bond length (position vector r (t)) and a bond angle for every unit time are shown, is shown in drawing 24. This data is inputted into the membrane-characteristics calculation unit III, and basic membrane characteristics (optical, electric, crystallographic characterization) are computed here.

[0234]About the process variation calculation unit I, an example of the two-dimensional general-purpose system is indicated to JP,H3-164904,A.

[0235]As for a three-dimensional process simulator, this artificer succeeded in construction this time. Below, it has drawing 8 and this is explained without moving from its seat. Art and structure of a simulator are surveyed first. Although an application concerned has put a subject on an atom level, it has also proposed a new uniting method with other process variation calculation units I, is effective and more exact, and also shows that the new function which the former has can also be provided. A process variation calculation unit (10) of a partner who unites is the three-dimensional process simulator Ic, for example, and belongs to what is called a fluid model. In particular, this invention persons describe below the contents of the three-dimensional process simulator Ic who built newly. The main point is those with two and connection with an atom level simulator be possible for a "three-dimensional process simulator" whom this invention persons built first. Next, into a portion of this "three-dimensional process simulator", this invention person etc. are making full use of a chemicals model conquered newly and a mathematical expression. By these, union with an atom level was attained for the first time. A viscoelasticity coefficient, a stress constant, a diffusing constant, Cij, etc. are one of those are outputted from an atom level simulator, and these are transmitted to a fluid general-purpose three-dimensional process simulator. In drawing 8, it is (23), (33), (43), (53), (63), (73), and (83). For example, diffusing constants, such as an oxidizer, are transmitted to (23). A method of transmission procedure is mentioned later. Conversely, from a fluid general-purpose three-dimensional process simulator, it is transmitted to an atom level simulator and these viscoelasticity coefficients, a stress constant, a diffusing constant, Cij, etc. can be complemented mutually. That is, more precise prediction is realized by calculating by both three dimensions and exchanging a three-dimensional result mutually.

[0236]By the general-purpose three-dimensional process simulator (10) side, calculation of process induction stress of an extensive field of several micron level according to input data by (2) and (3). More more exact functions can also be used by once transmitting a deed and this result to the molecular dynamics simulator II, or returning them to a general-purpose simulator (10) again via a file (22) and a file (32), and repeating this. Transmit a result of process induction stress calculation of a a certain grade extensive field which is a certain time, for example and for which it asked in a process variation calculation unit as a calculation procedure to the molecular dynamics simulator II, and once here, calculating a correction amount of a physical property value, anew, a motion of an atom is seen, a corrected physical property value is again sent into a general-purpose simulator, and results, such as process induction stress of an extensive field, are advanced by a general-purpose simulator. if sufficiently big stress is locally generated by repeating this, a motion of an atom can be seen by the molecular dynamics simulator II side, and propriety of plastic deformation can also be seen.

[0237]Of course at the time of impurity redistribution calculation in the above-mentioned general-purpose process simulator portion, and stress calculation, a point defect action calculation part (9) described in drawing 8 is called. As a point defect, a vacant lattice in a Si substrate and Si between lattices are treated. Unless it takes in an action of these point defects correctly for diffusion of an impurity, redistribution of an impurity is not calculated correctly. Of course in an ion-implantation calculation part (4), a lot of vacant lattices by pouring damage and Si between lattices are generated. Although the redistribution of these is carried out to midium like a heat process, an impurity must have an interaction and they must make it reflect in calculation of impurity distribution then. Of course also by silicide, shape, and a stress calculation part (7), a vacant lattice in a Si substrate and an action of Si between lattices must be considered enough.

[0238]by the way, drawing 8 — in addition to this, (8) is described for a few. At an LSI element trial

production process, as for oxidation, diffusion, an ion implantation, etc., each required physical property value is already stored in this process variation calculation unit (10) based on many data. For example, PB1 of a formula (1130) behind hung up about oxidation of Si and PB2 grade are it (1131). D' etc. of a formula (1531) which hangs up a diffusing constant of an oxidizer in SiO2 film behind are it. Generally, this appearance has data in general.

[0239]However, data etc. are not necessarily assembled in LSI development. For example, trial production development of the memory cell using a ferroelectrics film is considered now. A case where $PbTiO_3$ is formed is considered using CDV or a weld slag process. In the present general-purpose process simulator, yet, a diffusion coefficient of various impurities in inside of a $PbTiO_3$ film does not understand many so much, either, and the stress constant does not understand them so much, either. A segregation constant of an impurity in an interface is not known so much, either. In such a case, as it goes into a process of (8) first and is immediately shown in (84), it once goes to the molecular dynamics simulator II, and potential of a required element, etc. are computed, and a molecular dynamics portion moves there based on it, and a physical property value is computed. Although an already described portion is resembled very well after this, these physical property values are stored in a file from (83). And a calculation part is advanced like a process variation calculation unit.

[0240]Here, explanation adapted to concrete processing is given with reference to drawing 9. Here, an oxidation process is taken up. That is, a wafer is thrown in, this is moved to a substrate treating process, and it goes into after an appropriate time at an oxidation process.

[0241]Quantity of high purity oxygen gas is set to Pox, and distribution of this consists of this oxidation process as sigmatox, for example. ** and a temperature-up sequence are set to Temp, and constitute sigmatemp and a BARUPU sequence for distribution of this like tox and sigmatox. When having opened pulp, for example, a question is especially in a BARUPU sequence very here, but it is what was described in working example for details.

[0242]For example, in drawing 8, oxidation, shape, and a stress calculation part of (2) are accessed, and the partial pressure Pox, the temperature Temp, etc. are inputted here. And stress calculation is also advanced to oxidation growth calculation and coincidence. At this time, distribution / change calculation is also performed using (21). Here, sigmapox and sigmate ** input and a variations from a center value is calculated efficiently.

[0243]As for shape of an amount of growth of an oxide film, and an interface of an oxide film and Si, and also impurity quantity, these calculation results are calculated, for example. According to this invention person, stress is also called for. It is similarly from distribution and change. Shape of an amount of growth of an oxide film and an interface of an oxide film and Si and also impurity quantity are calculated also about Pox=Pox+sigma pox and portions, such as Temp=Temp 10sigmatemp. And these are once stored in a memory or a file (22), and are sent to a molecular dynamics portion. In a molecular dynamics portion, these are inputted as the signal a and position vector r (t) is computed.

[0244]Although drawing 10 shows the same distance figure as drawing 9, it is related with formation of a ferroelectrics film here.

[0245]By the way, explanation about a diagnostic portion in this invention is also given here. A part of binary tree by this example is shown in drawing 11. Here, a binary tree which paid its attention to an oxidation process is shown. As described also into a figure, SiO2 thickness sent from the in-situ MO 2 evening is first compared with SiO2 thickness predicted from calculation here. And it is taking up and arguing about a time of thickness being settled in tolerance level. If it does so, 1R SUBEKUTORUKAPU sent from an inlitu monitor is compared with 1R curve predicted from calculation as a following procedure. And as shown in a figure, first, a spectrum is compared and, moreover, a case where a spectrum shifts to the number side of Takanami is taken up by a case where it has shifted for a while. If it does so, it is possible as a following procedure that remaining stress has induced greatly in SiO2. Then, the temperature can be slowly lowered in this case and remaining stress can be made to reduce. Then, an annealing portion indicated to drawing 9 is corrected, and it is inputted into (2) of drawing 8. On the other hand, when comparing a spectrum and going into tolerance level, it continues with the original process sequence. When thickness is not settled in tolerance level, poor processing is performed as correction being impossible.

[0246]Data flow thinks in general that it understands now about drawing 8. I would like to make

reference about an output of drawing 8 to a slight degree. That is, an executed result is once stored in a file (3). Here, a spectrum corresponding to a process searched for at each process, and optical [other] and electrical property results are stored. Although these give details later, they can be contrasted with quantity which is monitoring as data measuring.

[0247]On the other hand, one person of this invention persons has proposed before a process simulator system which used variations calculation of a process variation. That is, they are JP,63-174331,A and JP,H3-164904,A. In these proposals, each process, such as oxidation/diffusion, an ion implantation, chemical deposition (CVD), etching, and lithography, can be dealt with by the handling like a fluid. For example, it is asking for redistribution of an impurity in a diffusion process by a fluid model, taking in an electric effect distinguishing an impurity total amount and electrical activation impurity quantity.

[0248]An outline of a simulation system shown in JP,63-174331,A and JP,H3-164904,A is explained with reference to drawing 25 - drawing 49. In these proposals, it is treating as follows about a process variation. When a process of oxidation, an ion implantation, and lithography is taken for an example, for example, an average temperature (T) and with the permission Bala (deltaT), The permission Bala, a mean pressure (P) and with the permission Bala (deltaP) (deltat) and also an average mask size (L) and with the permission Bala (deltaL), an average dose (D), with the permission Bala (deltaD), etc. are input values. [the average number of hours (t),]

[0249]As shown in drawing 25, a portion which calculates distributed change (deviation) to each subroutine, such as an ion implantation, oxidation/diffusion, and lithography, is attached to a process simulator. As a computational procedure, a method of calculating the variations and going is adopted, advancing calculation about these center values.

[0250]This variations calculation is explained a little. If a temperature variations in a diffusion process is explained first, in a diffusion process, epsilon and the number of electrical activation impurities are set to N for an internal field according a diffusion coefficient to D and impurity distribution, an equation based on the second law of Fick is solved, and the impurity atom concentration profile C is searched for. A procedure of variations calculation is shown using drawing 26. Here, let left-hand side in a figure be a normal process (Normal process).

[0251]A following formula (0071) can express a nonlinear diffusion equation.

[0252]
[Equation 92]
k and k+1 are time here, and impurity concentration Ck+1 at the time of the time k+1 is an unknown. B of the right-hand side originates in the 2nd paragraph of a following formula (1072).

[0253]
$$**C/**t->(C_{k+1}-C_{k})/t -- (1072)$$

Here, since an implicit method is used, a coefficient matrix which appears in an upper type is altogether expressed using D, the mean temperature T, etc. It is diffusion-time tn+1 in the case of a normal process predetermined. Even eye watch is divided suitably and it goes in quest of a solution one by one to t1, t2, --, tn+1. Here, in each time, t1, t2, --, tn+1, these were linearized using the Newton method, and calculation is recommended.

[0254]Next, a change process (Process deviated) is explained. Here, a case where change deltaT occurs to diffusion temperature is shown. When a variations of an upper type is taken and variation deltaCK of concentration in the time k is known, variations deltaCk+1 at a time of being the time k+1 is expressed by following formula (1081).

[0255]
[Equation 93]
That is, in the time k+1, the value D, psi, and N at the time of convergence of a normal process, C, etc. are saved, and F' is created using these, and the variation to the temperature T is prepared, and deltaCk+1 is calculated. Some matrix elements for creating F' here are shown in drawing 26. The hole model is fundamentally used for derivation of a diffusion coefficient. In this case, a Fermi level changes with temperature changes, the concentration of an electrification hole changes and a diffusion coefficient changes with these. Therefore, to the intrinsic carrier concentration ni which becomes the basis first, the variations comes to be shown in a following formula (1082).

[0256]

[Equation 94]

$$deltan_i = n_i(1.5/T + 0.605/kT^2) \, deltaT \quad -- (1082)$$

Change by the temperature of the internal field of an impurity can also be expressed using these. It took into consideration also to the variations of the increase phenomenon (Oxidation Enhanced Diffusion Effect) of the diffusion coefficient in an oxidizing atmosphere. In the oxidation process, since the linearity oxidation rate constant (Linear rate constant) and the parabola oxidation rate constant (paraboric rate constant) also changed, this was also taken into consideration. Previous F' is created using these.

[0257]Here, a certain typical diffusion process is taken up and the situation of convergence in the one diffusion time is shown in drawing 27. The horizontal axis of drawing 27 shows number of occurrence, and the vertical axis shows the remainder. The converging state in a normal process is shown by drawing 27. In a normal process, it turns out that it is converging by 3 times of Newton loop. Variations procession F' previously shown using D at the time of this convergence, psi, N, etc. is created, and a temperature variations is calculated. As shown in drawing 27, it turns out that it converged by about 50 times and has ended with 1/10 of the whole of computational complexity.

[0258]Drawing 28, drawing 29, and drawing 30 show accuracy of a variations. Drawing 28 expresses impurity distribution at the time of 1000 ** over a two-dimensional lattice as a normal process. Drawing 29 is a change process and is calculated based on drawing 28 by a case of deltaT=1 **. On the other hand, drawing 30 hammers out 1001 ** as a normal process.

[0259]value + drawing 29 of value = drawing 28 of these figures to drawing 30 -- a value -- it turns out that it is related. It turns out that it comes to be shown in drawing 31 when a value of drawing 30 is plotted anew, and it is in a tendency for impurity concentration to fall in the high concentration side if it shifts to an elevated temperature, and is in a tendency which increases in the low concentration side.

[0260]When creating a semiconductor device, there are many processes and there are two or more parameters in each process. For example, an ion implantation to the things main at a CMOS process, and a (i)N-well field, (ii) It consists of patterning of Si_3N_4 for an ion implantation to a P-well field, and a (iii)LOCOS process, a (iv)LOCOS process, a (v)n+ ion implantation, a (iv)p+ ion implantation, a (vii) annealing process, etc. When you consider fluctuation of a process, it is necessary to deal with change and frequency of many of these parameters (or frequency).

[0261]Frequency of a variations and combination of execution are considered by JP,63-174331,A and JP,H3-164904,A. Now, since it is easy, three processes, alpha, beta, and gamma, are considered. In each, a center value of a process parameter C (Center), A value displaced to U (Upper) and negative in a just displaced value was named L (Lower), and from JP,63-174331,A and JP,H3-164904,A, those frequencies were defined, as shown in drawing 32.

[0262]When the processes alpha and beta are considered, the combination can consider CU, UC, CC, LC, and combination of five pieces of CL, if calculation execution of UU, LL, etc. is disregarded. When passing through a process of gamma succeedingly furthermore, seven combination shown in a figure can be considered. However, he does not deal with these all but is trying to calculate from U in consideration of the symmetry of U and L in JP,63-174331,A and JP,H3-164904,A in L.

[0263]Some trees of search of an inference engine which is the central part of this system are shown in drawing 33. Here, oxidation and a diffusion process are examined. "**" in a figure shows a predicted value by a statistical analysis system, and a "fruit" shows an actual measurement.

[0264]An acceptable value used at this time is a value which passed through whole processes, such as oxidation, diffusion, and etching. At this time, epsilon value is obtained by performing a two-dimensional process statistical analysis system. when a "fruit" came out of "**" **epsilon, as shown in drawing 33, an oxidation process had abnormalities -- purport description is carried out. In this case, temperature or time performs a load module of a statistical analysis system for which had shifted if needed. The above-mentioned assay is performed also about a lithography process, although explained focusing on oxidation and a diffusion process. Fluctuation by a lithography process is equivalent to a lateral slip of shape of a SiO_2 film, a junction type-like lateral slip, etc.

[0265]Although Common Lisp is used for an inference engine, it is being suitable not only for numerical processing but processing of a text (List) and processing of shape, and because this is still very simpler

for maintenance of a system. This system not only reads data of an actual measurement from an inference engine, but is performing a load module of a statistical analysis system.

[0266]According to the simulation system shown in JP,63-174331,A and JP,H3-164904,A. A variation part can be processed now by computational complexity of the conventional abbreviation 1/100 by saving a coefficient of a procession at the time of convergence of normal repeated calculation in each process, and creating a primary variations procession using this, and taking into consideration change of each process parameter of said, and these crowdedness effects. By interlocking an inference engine and the above-mentioned system by Common Lisp, for example showed being made to a diagnostic pan of a process margin and also abnormalities in a process to optimization.

[0267]In JP,63-174331,A and JP,H3-164904,A, a basic diffusion equation is stood, as shown in a following formula (1111) to each impurity.

[0268]

[Equation 95]

Here, t shows time, x and z are coordinates of the horizontal direction of two-dimensional space, and the perpendicular (facing down) direction, and N is [C is impurity concentration and] electrical activation impurity quantity. D is a diffusion coefficient including concentration dependence and the enhanced diffusion effect, and a following formula (1112) can express it.

[0269]

[Equation 96]

Di is a basic diffusion coefficient independent of concentration among a formula, and the temperature dependence is expressed by the following formula (1113).

[0270]

$D_i = BB$ and $_{exp}$ (-BA/kT) -- (1113)

The constant according [BB and BA] to the kind of impurity and k are Boltzmann constants. FE is given with a following formula (1121) by making ni into intrinsic carrier concentration.

[0271]

[Equation 97]

n is 1/2 $[(C_D-C_A) + (C_D-C_A)^2 + 4n_i^2]$. Furthermore, it is ni,[Equation 98]

$n_i = 3.87 \times 10^{16} \times T^{1.5} \times _{exp}$ (-0.605/kT)

-- (1122)

It carried out.

[0272]An oxide film growth rate was expressed as shown in a following formula (1123) and (1124) using the parabolic nature oxidation rate constant R1 and the linearity oxidation rate constant R2, respectively.

[0273]

R1=PB3and$_{exp}$ (PB1/kT) -- (1123)

R2=PB4and$_{exp}$ (PB2/kT) -- (1124)

When the above-mentioned parabolic nature oxidation rate constant is anew described as B and B/A, there is a relation which sets Zo and oxidation time to t and shows oxide film thicknesses in a following formula (1125) by making tau into a constant in respect of the horizontal coordinates x.

[0274]

These are prepared and it asks for a variations to temperature deltaT of each above-mentioned coefficient.

[0275]A variations of n comes to be shown in a following formula (1131) as deltani =ni and (1.5/T+0.605/kT2) deltaT.

[0276]

[Equation 99]

A following formula (1132) is materialized.

[0277]

[Equation 100]

The variations of a growth coefficient is expressed by a following formula (1133) and (1134).

[0278]

[Equation 101]
When it rewrites to B=R1, A=R1/R2, it comes to be shown in a following formula (1141) and (1142).
[0279]
[Equation 102]
And the variations of t+tau becomes like a following formula (1143).
[0280]
[Equation 103]
The simulation system explained above was epoch-making as that time. It is impossible however, to already use for the process control and monitor art in the latest clustering tool.
[0281]Then, this invention persons repeat examination further and came to complete this invention. Here, optimal design of the ferroelectrics film of the electric field effect type MIS element which used the perovskite single crystal was performed, the element was actually made as an experiment and evaluated according to this, and invention completion was checked.
[0282]Namely, being provided by Claim 11 is in charge of forming an electric field effect type MIS element on a semiconductor single crystal substrate, In a system which uses a ferroelectrics film of this MIS element as a single crystal, and moreover contains this semiconductor substrate and this single crystal ferroelectrics film, It is a manufacturing method of an electric field effect type MIS semiconductor device considering it as design arrangement of a single crystal ferroelectrics film and a substrate which introduced a ******** valuation function into abinitio molecular dynamics theory expressing the object characteristic, and followed the optimal solution of a system under desired main movement conditions by this.
[0283]Being provided by ** and Claim 12 is in charge of forming an electric field effect type MIS element on a semiconductor single crystal substrate, In a system which uses a ferroelectrics film of this MIS element as a single crystal, and moreover contains this semiconductor substrate and this single crystal ferroelectrics film, abinitio molecular dynamics theory expressing the object characteristic of the system — as a ******** valuation function — a system — it is a manufacturing method of an electric field effect type MIS semiconductor device arranging said single crystal ferroelectrics film so that the whole free energy may be taken up and free energy may become the minimum under main movement conditions.
[0284]Being provided by Claim 13 on Si semiconductor single crystal substrate, In forming an electric field effect type MIS element, a gate insulation oxide film of this MIS element is used as a single crystal, and abinitio molecular dynamics theory which expresses the object characteristic of the system in a system containing this semiconductor substrate and this single crystal ferroelectrics film — as a ******** valuation function — a system — the whole free energy, [take up and] This free energy is a manufacturing method of an electric field effect type SiMIS semiconductor device arranging said single crystal ferroelectrics film under main movement conditions so that it may become the minimum.
[0285]Being provided by Claim 14 on Si semiconductor single crystal substrate, In forming an electric field effect type MIS element, a gate insulation oxide film of this MIS element is used as a single crystal, and abinitio molecular dynamics theory which expresses the object characteristic of the system in a system containing this semiconductor substrate and this single crystal ferroelectrics film — as a ******** valuation function — a system — the whole free energy, [take up and] While this free energy arranges said single crystal ferroelectrics film so that it may become the minimum under main movement conditions, it is a manufacturing method of an electric field effect type SiMIS semiconductor device stopping oxygen deficiency concentration of that single crystal ferroelectrics film to 0.01% or less.
[0286]Being provided by Claim 15 on Si semiconductor single crystal substrate, In forming an electric field effect type MIS element, a gate insulation oxide film of this MIS element is used as a single crystal, and abinitio molecular dynamics theory which expresses the object characteristic of the system in a system containing this semiconductor substrate and this single crystal ferroelectrics film — as a ******** valuation function — a system — the whole free energy, [take up and] While free energy of this system arranges said single crystal ferroelectrics film so that it may become the minimum under main movement conditions, It is a manufacturing method of an electric field effect type SiMIS semiconductor device, wherein unevenness of local energy dedicated within deviation score 3sigma and stops oxygen deficiency concentration of the single crystal ferroelectrics film to 0.01% or less

especially.

[0287]These optimization procedures and a trial production result are described below.

[0288]Here, as a single crystal ferroelectrics film, PZT system perovskite was taken for an example, for example, and a Si surface was made into a field (100). Cu of FCC structure may be sufficient as this substrates face as a metal electrode. The most important problem is transposed to a problem to what kind of crystal physical relationship single crystal ferroelectrics film PZT system perovskite and Si (100) side should be arranged. Here, total energy of a system was taken up as a valuation function which is a main point of this invention. And a Si/PZT interface was taken up as this system. Perovskite as PZT under impression conditions and physical relationship of Si (100) found out that it was optimal to perform it as follows by this invention persons' creating an energy expression as a strict valuation function beforehand, and using this. That is, the median line of an angle a1 axis of C4v structure expression of perovskite and a biaxial to make was aligned with [110] shaft orientations on Si (100) side, and c axis was leaned, and coinciding the 1st Si and the 3rd Si position with Si on Si (100) side found out that it was an optimum value. At this time, it was also simultaneously shown in PZT that less than 0.01% of oxygen deficiency is tolerance level. A key map which this invention created to this appearance proposes was shown in drawing 34.

[0289]It is attached to drawing 34 and explains in detail. An upper half of drawing 34 a shows a top view of a simple lattice by the side of Si, and a lower half is sketch drawing of a PZT side. It is indicated that drawing 34 c is best to arrange in parallel a line which ties perovskite to the direction of [110] Si. Although explained for details later at this time, in order for a straight line connected to silicon to become parallel to [110] Si, C axis of perovskite needs to incline. By carrying out like this, according to this invention persons' calculation, a line which connects Si to perovskite was only arranged in parallel, and it also found out that total energy fell 10 more% compared with a case where C axis is not leaned. When use for an element was further actually considered by besides and it was in PZT even within 0.01%, it found out that the original feature of single crystal perovskite was shown enough.

[0290]A problem of surface energy pointed out here affects an element characteristic plentifully so that it may explain below. An azygos atom will be made easy to form and energy by mismatching generated in an interface which a ferroelectrics film and a substrate form will promote formation of interface state density by this. This interface state density leads to hindrance of a conduction phenomenon, and a fall of reliability. A defect of an unusual bond etc. was made into a film and a possibility of becoming level is conceived. Here, tolerance level of these defects is shown for the first time.

[0291]Comparison with the MIS characteristic and a conventional example which were created by this invention was also performed. A CV method was used especially here as what can evaluate interface state density effectively. Dispersion in data was also correctly shown in the characteristic by this invention. When based on this invention, it turns out that a value is falling to 10 by about 1/at the interface state density compared with a conventional example. When mobility of an MIS element by this invention was also evaluated under the same electric field situation, about 12% of improvement was found. Reliability also improved.

[0292]A procedure which came to invent the axial new relation which this invention persons do not have until now is explained in more detail. Drawing 35 is structural drawing of completely new strict abinitio / molecular dynamics simulator which this invention person etc. created. An upper half of drawing 36 is a portion of abinitio, and a lower half is a portion of a molecular dynamics simulator. using this simulator -- for the first time -- artificers -- for example -- Structure of perovskite showed what kind of thing it was. Drawing 37 is the first perspective diagram of perovskite in which this invention persons were able to show a strict structure. A large ball in a figure shows oxygen and a small ball shows Pb. Since it is a field complicated to this appearance which field of perovskite and which field of Si carry out **** junction as the Z-axis shows C axis of perovskite here and it understands by a diagram, it turns out extremely well that a guess is difficult.

[0293]Paying attention to an oxide film, contrast work of spectrum data was done as an accuracy check of the above-mentioned molecular dynamics simulator. That is, ROKKIN mode, stretching mode, etc. of O-Si-O or Si-O-Si were sometimes read in a position of Si atom of ****, or an oxygen atom, etc., and undamped natural frequency was calculated from these figures. When this is compared with an actual measurement, it is 490 cm-1 and 1111 cm-1 to 440 cm-1 and 1100 cm-1, and is an appropriate range, respectively. When a pressure was impressed, it also turned out that it is well in agreement with an

actual measurement that intensity in O–Si–O mode increases.

[0294]This invention persons calculated also about a case where very big compression stress is impressed to PZT, also recommending such inspecting work. As an interface, a way which took such a structure also understood that there was a profit of total energy.

[0295]A field etc. which were used for calculation are discussed in detail a little. In calculation, to the Si–substrate side, tens atomic layers were taken to a depth direction, tens atomic layers were taken to a depth direction in the surface, and tens atomic layers were taken also to a longitudinal direction, and a calculation area was taken. Also in perovskite, ten atomic layers of numbers took height in every direction at a time, respectively.

[0296]It can be gathered by this method that new physical relationship was able to be found out by a technique twisted until now. This invention persons developed a strict addition type of strict ionic bond potential to a field containing a ferroelectrics film and a Si single crystal. In the conventional technique, stringency was missing, especially energy of a system was not able to be searched for correctly. In this Description, this invention person takes the side of a conventional fault and an inaccurate place, one by one, clarifies and goes.

[0297]According to this invention person, it can explain as follows. This invention persons built the new simulator which is not in the former, and calculated about perovskite on a single crystal of a ferroelectrics film, and a concrete target as an example.

[0298]Explanation is added a little, carrying out comparison with the former to below also about a simulator which this invention person created. For example, an oxide film is described first. Three kinds of potentials, between Si–O, between O–O, and between Si–Si, must be expressed strictly. Potential of total between Si–O, between O–O, and between Si–Si will be very difficult in practice, and all three sorts of amounts of addition will be infinitely emitted by a paragraph of the distance r. Since the Coulomb potential lengthened the skirt to a distance, the calculation itself could not close it, but it was using a method of Ewald by the conventional technique in somewhat strict calculation. However, although mentioned later, stringency is lacked in calculation.

[0299]In actually arranging, a technique which this invention persons used is shown below. Here, this invention persons show the first simulator to create below.

[0300]This invention persons built an original new abinitio molecular dynamics system, though it inquired wholeheartedly and computational physics was followed. It is why a new trial became possible just because there was this new system. What this invention person etc. created below is explained in detail.

[0301]Although SiO_2 was taken for an example here, about other things, it also checked that it could be used only by replacing a number of an element, etc.

[0302]An entire configuration of the new simulator which this invention person etc. proposed is described in drawing 38. The new technique of having compounded a molecular dynamics portion (MD) and a density functional (DFT) was proposed. Proper use with a molecular dynamics method and a density functional method by this invention persons is shown below first, using drawing 39.

[0303]As shown in drawing 36, a molecular dynamics (MD) portion occupied a lower half of a flow chart, and a density functional portion (DFT) occupies an upper half. a molecular dynamics method does not come out OK -- the so-called a little big system in limited temperature is treated, and potential beforehand searched for from the ultimate cause is used for potential between atoms (ion). On the other hand, a density functional (DFT) was made to use, when searching for a ground state of a small system. And naturally a portion of DFT set temperature to 0K. It asked for a potential portion from a ground state of an electron system. A wave function (KS equation) was specifically solved and a partial density functional was used together.

[0304]Calculation procedure of a simulator by this invention person etc. is actually explained taking the case of Si and O. It asks for total energy of a ground state of an electron system without degeneracy in a DFT portion, and is **. [External Character 1]
It is].

[0305]namely[Equation 104]
[External Character 2]
N interaction energy and the 3rd paragraph are kinetic energy in case there is no interaction between

electrons supposing electronic one-body approximation,[Equation 105]
It is written. The 4th paragraph is exchange correlation energy and the form is based on partial density approximation. **[External Character 3]
[Equation 106]
[External Character 4]
Equation (Kohn-Sham equation)[Equation 107]
[External Character 5]
It must solve self-contradicting [no] (self-consistant).
[0306]
[External Character 6]
It applies and integrates with the electron density n to RUGIepsilon$_{xc}$ (n),[Equation 108]

It carried out. The form of epsilon$_{xc}$ (n) is proposed variously the formula besides Wigner etc. Further,

[External Character 7]
A ** Coulomb field is not used as it is, but it sets by the norm preservation pseudopotential which erased the singularity in the nuclear position, and is a frog. The number of the ingredient in the Fourier expansion was able to be pressed down by accustoming in this way.
[0307]As total energy, this invention persons use the thing also containing the coulomb potential between atoms (ion) in order to expect ****. namely[Equation 109]
[External Character 8]
epsilon etc. . A formula (2071) to the 1st paragraph of the right-hand side is the right from the formula (2065) of DFT.[External Character 9]
It comes out. The portion is Veff from the formula (2065) of one-body approximation like the case of DFT.[External Character 10]
A new view was put in here. It considers that E is potential energy and is kinetic energy virtual otherwise.[Equation 110]
It introduces. Therefore, a Lagrangian is L=K-E. -- (2073)
M_I in a formula (2073) are mu and mu although it is the mass of a true atom (ion). It is virtual mass and changed according to the purpose like the after-mentioned. They are regular rectangular cross conditions as a binding condition. [Equation 111]
Since it ****, when making the Eulerian equation, undetermined-multipliers lambda$_{ik}$ is introduced, and it is L.[Equation 112]
The variations of *********** is taken. The result[Equation 113]
The temperature T of the kinetic energy of a formula (2073) corresponds. If it says by a relation with sigma1/2$M_I R_I^2$, it will be a temperature that it is not virtual and actual, because the degree of means has temperature each one by the energy equipartition law of classical statistical mechanics. mu and mu nu$_i$nu can be controlled or reinforced by size.
[0308]For example, if it is referred to as T->0 from an elevated temperature as mu M_I, psi$_i$ will change with R_I stopped and a ground state of an electron system will be acquired. The left side of a formula (2076) is set to 0 at this time, and the right-hand sides are a formula (2071) and the cautions under it. [Equation 114]
Since it becomes, {lambda$_{ik}$} which makes the linear combination of psi$_i$ suitably is diagonal-line-ized, and obtains a KS equation (2064). That is, it means obtaining the same result as having solved the KS equation by DFT by simulated annealing. However, although the state of the temperature T is made, since it was not based on the Monte Carlo method but movement of the virtual dynamical system is followed, it is called dynamical simulatedannealing (DSA).
[0309]When integrating with a formula (2076), psi$_i$ cannot necessarily be treated as a variable as it is, but the expansion coefficient (that is, Fourier coefficient) which developed it by the plane wave can be treated as a variable. In order not to increase the number of this expansion coefficient recklessly, it is required like the case of DFT to erase the singularity in a nuclear position at pseudopotential. When especially the periodicity of a crystal can be used, the linear combination of psi$_i$ which diagonal-line-izes

above {lambda$_{ik}$} is described as phi$_{nk}$. k is a wave number vector in a Brillouin zone, and n is a zone index.

[0310]phi$_{nk}$[Equation 115]

******** is **. lambda$_{nk}$ is a characteristic value of a procession {lambda$_{ik}$} and is an energy level. phi$_{nk}$ (ₙ, t) is developed.[Equation 116]

[External Character 11]

Effective potential V$_{eff}$ which is not filled is also developed.[Equation 117]

A formula (2075) and a formula (2076) are substituted for a formula (2074).[Equation 118]

[External Character 12]

It becomes common, so remove.[Equation 119]

******. Since this formula is clearing up the integration of the vibrating part analytically, purely, rather than a numerical method, it can enlarge deltat and can decrease computational complexity.

[0311]The Coulomb potential is as follows. this invention person found out being divided into the 4th paragraph, when it decomposed. Although there was only the 3rd paragraph in particular conventionally, it checked that there was the 4th paragraph newly. These methods are described one by one. As shown below, this invention persons began to solve these as a start of a strict formula first from a basic equation which considered a dielectric constant. It is a basic equation first.

[0312]

[Equation 120]

a conductor -- epsilon=infinity and in the case of the vacuum epsilon= 1, the Coulomb potential differs, L is taken by 1 ** of a unit crystal (cube), sigma is taken within a unit crystal, and it is electrification and the position of Zi, and the oxygen i i-th particle. This is because polarization arises in the inner surface of a ball by electrification in a ball. Although the layer of electric doublet is made in the inner surface of the ball which is not a conductor, the last paragraph of the above-mentioned formula serves to negate the effect exactly. Since the method of Ewald gives the thing of the left side and epsilon=infinity, it must add the last paragraph of the above-mentioned formula in quest of the value within a vacuum. Only a result is hung up. The conventional derivation often has an error also in this portion.

[0313]Coulomb potential[Equation 121]

[External Character 13]

It set up as follows.

[0314]

[Equation 122]

It is expressed. n$_x$, n$_y$, and n$_z$ are the vectors of Tooru of x, y, and the direction of z here, respectively, and n$_x$, n$_y$, and n$_z$ are the integers ranging from −infinity to +infinity, respectively (in the case of a bulk crystal). It shall mean that ' of sigma' removes j=i at the time of n=o.

[0315]New F function is introduced here,[Equation 123]

[External Character 14]

It ********(ed).

[0316]This invention persons transform this still as follows, [Equation 124]

Index m$_x$, m$_y$, and m$_z$ are the integers ranging from −infinity to infinity, respectively. = At the time

[External Character 15]

[Equation 125]

[External Character 16]

[Equation 126]

*******.

[0317]The Coulomb potential which this begins, [Equation 127]

[External Character 17]

[Equation 128]

This Since it does not contain, it is not related to power. It can change still like the next.

[0318]

[Equation 129]
summarizing the result of former -- coulomb potential -- after all[Equation 130]
[External Character 18]
It is $/L_x$, 0, and $0+m_y$(0 or $1-/L_y$, 0)$+m_z$ (0, 0 or $1-/L_z$). The good point of the condition of the above-mentioned expression is that decrease by the factor of erfc in phi (1), and the paragraph of sigma declines quickly by the factor of exp by phi (2) to the paragraph of sigma of a basis declining only to the order of a reciprocal in the paragraph of sigma. Since it is effective for reverse at slowness and fastness with attenuation by phi (3), suitable kappa which can balance both is chosen. It is the result of calculating contribution of Coulomb force sequentially from the near place of distance, and is a result in case the circumference is moreover a conductor. according to the case where the circumference is a vacuum -- already -- the 1st paragraph is added. Especially this is the portion which was not considered conventionally.

[0319]A point-of-rotation group which this invention person etc. created is shown below using drawing 40. Si atom is put on the center (0, 0, 0) of a ball of the radius r, and four oxygen atoms are put on a position of the peak of a surface-of-a-sphere top regular tetrahedron. A position of C atom can be specified by an Eulerian angle (theta, phi). What is necessary is to face a vector (0, ogamma) which goes to the North Pole, and just to carry out rotation of the circumference theta of the y-axis, and rotation which is subsequently the circumferences phi of the z-axis first, in order to express it with coordinates (x, y, z).

[0320]The rotation procession, [Equation 131]
When one of four oxygen atoms is put on the North Pole (0, *), and moreover when [here / phi is unfixed and] *, the position of other three oxygen atoms, being undecided -- an angle -- psi -- respectively -- (-- 109 -- degree -- 28 -- ' -- psi --) -- (-- 109 -- degree -- 28 -- ' -- psi -- +-- 120 -- degree --) -- (-- 109 -- degree -- 28 -- ' -- psi -- +-- 240 -- degree --) -- expressing -- having . Therefore, those (x, y, z) coordinates are formulas (2061), and costheta=-1/3, sintheta=2 root (2) / 3, and the thing that made phi psi, psi+120 degrees, and psi+240 degrees, respectively are made to act on t (0, 0r). [Equation 132]
It becomes. What is necessary is just to make R (phi, theta) of a formula (2061) act as it is, in order to make the 1st oxygen atom that had pointed out the North Pole direction of (theta, phi). As a result, this invention persons asked as follows. Coordinates (x, y, z) of four oxygen atoms, [Equation 133]
It becomes. Coordinates (x, y, z) of four Si atoms in a unit cell are expressed with the parameter a, b, and c. When it compares with drawing 40, 2a is a cycle common to a lengthwise direction and a transverse direction.

[0321]
(I -- 0, 0, and 0II III(a, b, c) (a-b, a+b, 2c) IV V (-b, a, 3c) -- that is (0, 0, 4c), The 1st atom is set at the starting point, and if a z-coordinate goes up constant value every c and carries out orthogonal projection to a field (x, y), a square is made by I, II, III, and IV. A z-coordinate 4c Increases by the 1st atom of the following unit cell, and the 5th atom is in atom [1st] right above. 90 degrees of arrangement relative to Si atom rotate at a time to a circumference of the z-axis, and arrangement of four oxygen atoms belonging to each Si atom goes. Movement of the above Si atoms is added to it. What is necessary is just to use coordinates (x, y, z) of four oxygen atoms of the circumference of the 1st Si atom as it is, and a formula (2061) coordinates (x, y, z) of an oxygen atom around the 2nd, 3rd, and 4th Si atom, R (0, 90 ″) rotates to an oxygen atom of the circumference of the 1st atom, respectively. Rotation of the parallel translation R of (a, b, and c) (0,180 degrees) Rotation of the parallel translation R of (a-b, a+b, and 2c) (0,270 degrees) It will be obtained if parallel translation of (-b, a, and 3c) is made to act.

[0322]In addition, although a group of I II1, III2, II III1 and IV2, and III IV1 and V2 is the respectively same oxygen atom, these give the same expression of relations as a top (it is natural). The oxygen atoms I1 and II4 have shifted to a transverse direction by the one cycle 2a.

[0323]When it had investigated to this appearance, it investigated about whether a process is further actually considered and it approves to defect density of how much. That is, now, for example, 3200 Si, and 3200 Ti were prepared, and 100 oxygen deficiencies were made from zero piece to this. this case -- the next has sometimes comprised a position of Si atom of ****, or an oxygen atom, etc. clearly. First,

relation of dynamic behavior of an oxygen atom and Ti atoms and a PZT structure factor was investigated. When an oxygen deficiency exists in the single crystal PZT, as compared with a case of being defect-free, turbulence is clearly received to distant Ti and oxygen of the Kazuhara child point, and, moreover, mobility of a point defect is a very large thing. It turned out that a direction in PZT is size very much about such dynamic behavior compared with a case of single crystal Si also in influence and a range. There is an ionic bond ingredient in PZT considerably, and characteristically it is easy to polarize in it, therefore a local deficit grows into a trigger, and such an active motion is also considered to be interlocked with potential change. This invention persons were such procedure, and when were investigated in detail, and they were 0.01% or less, they found out that an advantage of a single crystal ferroelectrics film could be pulled out enough.

[0324]Below is used about atom level calculation of a ferroelectric material by this invention person. This invention persons advanced PTO, structure grasp with an atom level of PZO and PZT, and grasp calculation with structure and membrane characteristics. A result of calculation is reported. As an object structure of using by atom level calculation, (1) With what has oxygen and Ti in the high position of symmetry with a perfect crystal of PTO, respectively, and a perfect crystal of (2) PTO. Oxygen is what (drawing 37) put an oxygen deficiency into one portion which met at c axis at thing shifted and the 0.3A(3) above (2), a thing (drawing 43) which put an oxygen deficiency into (4) above (2) at one portion which met at an a-axis, the thing which replaced T of (5) PTO at Zr, etc. In particular, in (5), what replaced Zr in layers artificially was performed. It turned out that work of oxygen and Pb differs by PTO, PZO, etc. for the first time. From these, a cause of "spontaneous polarization" of a ferroelectrics film has been held. Relation of an atomic arrangement of a ferroelectrics film, distortion, deficit structure, etc. and basic membrane characteristics has also been held.

[0325]Calculation with an atom level of the most fundamental $PbTiO_3$ film is shown first. About a case where hauling distortion is received, a case (drawing 44, drawing 45) where Pb position is able to be shifted from an equilibrium point for a trial, a case where it has an oxygen deficiency, etc., when searching for membrane characteristics, it was investigated whether electric charge distribution which is to foundations most could be found well. Drawing 44 is a picture of a unit cell of $PbTiO_3$, and is a case where Pb is able to be further shifted a little from a center position. It asks for an isoconcentration figure of electric charge distribution at this time. Although drawing 45 is a unit cell too, it is a case where a portion of Ti-oxygen bond is made distorted. This result has shown the following points. (i) The whole has dramatically many ionic bond ingredients. It turned out that most electric charges can draw almost near to oxygen with strong (ii) electronegativity, and then the surroundings of Ti have an electric charge. (iii) -- although electric charge distribution is symmetrical and spontaneous polarization cannot happen the way things stand, considering oxygen "deficit" and position changing of Ti, it turns out easily that local electroneutrality is broken. Furthermore by hauling, it has also checked that a dielectric constant fell.

[0326]The following things were understood in a calculation result when it furthermore saw at 25 ** noting that there was no thermal agitation. That is, stable structure of PbTiO3 ideal film which consists of the point group C4v was searched for. As a result, even if it shifted oxygen very only, it turned out that it returns to the point group C4v of origin with stable energy. Is there any more stable equilibrium point as it usually says also at a place which was still larger and shifted 0.3A of oxygen positions? This was investigated. It is becoming still more stable toward a position which is distant from 0.3 A of starting points very only. In a position usually said, this neighborhood is said for this gap, therefore spontaneous polarization to arise. It turned out that what has a stabilizing point in those with at least two and a cubic position with simple one, and another are the positions a little shifted for the first time.

[0327]The origin of polarization is locally replaced also with an atom position which breaks down "neutrality" of charge quantity being a stabilizing point in free energy. In the above calculation, it turned out that existence of oxygen is very large. So, when carrying out an oxygen deficiency by accident, it turns out that it can become a big trigger also in crystal and electronically. (1) -- it seems that localization of the electric charge distribution is carried out to three kinds each of atoms, respectively [namely,]

[0328](2) According to an order in the periodic table O, and Ti and Pb, , respectively (2 or 2 s2 per s, two p4), it is (2 or 2 s2 per s, two p6, 3 s2, three p6, 3d2), and (2 or 2 s2 per s, two p6, 3 s2, three p6,

10 or 4 s2, four p6, 14 or 5 s2, five p6, 10 or 6 s2 and six p2). A thing especially with a large electric charge distribution area of Pb is known reflecting this.

[0329](3) When it sees well, divide and, as for electric charge distribution of Ti, it is in sight that the next O becomes irregular immediately.

[0330]In order to deter this, it turned out that there is also a hand which replaces halogens, such as F, Cl, Br, and I, well.

[0331]example 2 In upper example, although described about Si-PZT, a spinel $MgAl_2O_4$ film, cerium oxide CeO_2, and strontium titanate $SrTiO_3$ can also be used as a single crystal ferroelectrics film. Aluminum oxide $aluminum_2O_3$, zirconium oxide ZrO_2, and yttrium oxide Y_2O_3, yttrium stabilization zirconium YSZ, PrO_2, and calcium fluoride CaF2 etc. can also use the cascade screen. It is possible to apply modification which sandwiches the silicon PZT also in structures other than this example to an interface with this single crystal ferroelectrics film, a ground silicon wafer, or a foundation electrode.

[0332]If it is important to make free energy under voltage small and its attention is paid only to distorted energy, it is not necessary to be necessarily the minimum then. It is also based on thought that we showed perovskite.

[0333]A actual system of measurement by this invention is also explained. Drawing 47 is a circuit of saw YATAUWA. A circuit of this method is explained. As for a high voltage transformer and Co, known fixed capacity and CRO of T are cathode ray oscilloscopes. If Co is chosen more greatly enough than capacity of a ferroelectric sample, most of secondary voltage of T will start a sample, but since it is suitably divided by the resistance Rd and is added to a horizontal axis of CRO, deflection of a horizontal axis of CRO is proportional to the electric field E in a sample. On the other hand, although deflection of a vertical axis of CRO expresses voltage between both terminals of Co, this is equal to DS/Co. That is, a figure of CRO expresses a D-E curve and an absolute value of D and E is also easily obtained from deflection of a vertical axis. The spontaneous displacement Ds is obtained as D when outside looks for a saturation portion to E= 0, and the spontaneous polarization Ps is decided by Ps=Ds. If paraelectrics without a loss are observed in this circuit, it will become a straight line which passes along the starting point, but a case where there is a loss, and a ferroelectric have hysteresis. A D-E curve which becomes this invention was expressed with a solid line to drawing 48, and a dashed line showed a result of the conventional PZT to it for comparison. What becomes this invention is understood that a dielectric constant is also dramatically large so that it may understand from now on.

[0334]It is a place pointed out here at the impression time, and it tends to make the minimum energy by mismatching generated in an interface which a ferroelectrics film and a substrate form. And a thing on use was actually considered on this condition, and tolerance level of that quality was also shown. Reducing this surface energy leads to formation deterrence of level which becomes the hindrance of a conduction phenomenon, and improvement in reliability. According to this invention for this structure, it predicts by new abinitio / molecular dynamics simulator. Since any experiential model is not used for abinitio / molecular dynamics simulator which carries a desired valuation function, all places pointed out to this system can predict a natural phenomenon thoroughly. Here, also about a design, although an example which paid its attention to total energy at the time of impression of a system is shown, if it is a problem of a request of degradation deterrence, a design suitable for it will be attained further that a dielectric constant should be made a desired value, for example.

[0335]How to calculate the physical properties of the two-dimensional above was shown. An example of a calculation method of three-dimensional physical properties was already explained with drawing 8.

[0336]It is likely to be closed how **, and actual contrast and diagnosis are performed. That is, a simulation result is transmitted to a scheduler (13). At this time, from another side and a actual experiment system, monitor data is sent every moment and it comes. And data transfer from a file (4, 3) is synchronized with a thing with a scheduler as if these are stored in a file (4). And it is transmitted to contrast and assay / diagnostic block in the contrast diagnostic assay part IV.

[0337]In a clustering tool used for this invention, drawing 49 is a key map showing how an in-situ monitor measuring device is added. As shown in drawing 49, for example, it is input gas composition analysis, a XPS signal, a FT-IR signal, etc., these are the average value in predetermined time space, and the amounts of monitors are a part of mere information. This invention persons provide a method of

making a ************* measurand and sufficient information acquired from another side calculation contrasting. These are displayed as a picture [graphics / on a monitor] like drawing 50.

[0338]Drawing 51 shows a temperature sequence as an example of input data to an abinitio molecular dynamics simulation system by this invention. Drawing 52 shows a concept of atom level execution prediction by an abinitio molecular dynamics simulation system by this invention. Thus, a reaction on a substrate, dissociation of a molecule, etc. are describing, for example with an atom level.

[0339]Drawing 53 is a visualization figure of atom level execution prediction obtained by an abinitio molecular dynamics simulation system by this invention. After amorphous Si deposits this, it sees the state where it annealed at an about 600 ** elevated temperature, with an atom level.

[0340]An abinitio molecular dynamics simulation system of this invention is applicable also not only to Si but an oxide film. That is, drawing 54 shows an example of execution about SiO_2 of an abinitio molecular dynamics simulation system by this invention. Here, a Si-O-Si angle in SiO_2 is called for every moment, and a spectrum of FT-IR is searched for only by calculation by carrying out the Fourier transform, asking for character frequency from now on, and superimposing this. using this prediction result -- an actual measurement -- what is necessary is just to carry out comparison assay with data every moment

[0341]Drawing 55 shows an example of execution in an atom level using a simulation system of this invention at the time of using input data of drawing 51 shown previously. Drawing 55 shows performing as expected.

[0342]From drawing 56, even if, as for drawing 69, annealing from membrane formation of a Si film at the time of using input data of drawing 51, distance between Si-Si which can be further set by solid phase growth, and a bond angle change time and temperature, it stops.

[0343]In a system shown in drawing 1, basic membrane characteristics were computed in the membrane-characteristics calculation unit III. However, like a system shown in drawing 70, the special membrane-characteristics calculation unit III may be omitted, and the required characteristic may be computed inside process variation calculation unit I. They are deformable suitably according to a request of a design.

[0344]As mentioned above, it became possible to reduce hardware and computational complexity substantially by this invention as compared with the former. For example, speaking of computational complexity, by the process simulator TOPAZ, as shown in drawing 98, a memory is about 24 M bytes and execution time becomes for several minutes. On the other hand, in process simulator SUPREM4 [famous], since viscoelasticity etc. are taken into consideration, a memory amounts to 200 M bytes or more, and execution time will reach with clay also on the 1st. If it furthermore becomes molecular dynamics and ab-initio calculation, a memory has reached several times also several times and execution time.

[0345]In such a situation, molecular dynamics and an ab-initio tool will be used for full, and prediction of atomic dynamic behavior and prediction of optical various characteristics will be started [whether cost of a computer is large, and]. This invention persons also find out the new use art of a simulator by this art while finding out a method of making full use of mathematical new art, and conquering these disadvantages.

[0346]Conventionally, there are some which added some procedure above. It is a flow plan shown in drawing 99, and shows a main part of a flow of a density functional in the conventional molecular dynamics simulator. That is, in this technique, virtual mass is given and a Lagrangian of the whole system is used. This corresponds to a formula (1223) which this invention person etc. described previously. This is equivalent to the Car-Parrinello method already known. It is supposed that it is calculable of this method at a high speed apparently. However, a supercomputer of for example, a clay company level or calculation in one also still takes one whole day and night. Therefore, if 1-time calculation [1 time] was done in order to investigate change of various parameters, it cannot become a diagnostic tool in real time at all.

[0347]In order to actually work a process unit, appropriate preparation and expense start. According to this invention, without building a semiconductor manufacturing system and actually advancing a creation process of a semiconductor, only a process simulation or a thought experiment can be conducted and this is dramatically useful. For example, it becomes possible about looking for a new material easily and

effectively moreover by conducting a thought experiment using various molecular structure models, and predicting the characteristic of a device using it.

[0348]Drawing 131 is such a process simulator's lineblock diagram, and An input means of the internal memory means 3, such as the computer 1 and a hard disk drive, the mouse 5, the keyboard 6, etc., It consists of external storage of an output means of the monitor 7, the printer 9, etc., and CD-ROM11 and floppy disk 13 grade, and its drive drive 15.

[0349]A program which described procedure for performing a molecular dynamics simulation beforehand is created and stored in the internal memory means 3. This program is created by high-level languages, such as FORTRAN and the C language, combining assembler language as occasion demands, for example. Of course, such a program saved beforehand at external storage, such as CD-ROM and a floppy disk, may be suitably installed in the internal memory means 3.

[0350]Although processing performed here is the same as what was already explained, Interface Division with a semiconductor manufacturing system which is actually working is omitted. That is, only processing corresponding to a loop including the molecular dynamics simulator II of drawing 1, the file 1, the process variation calculation unit I that calculates broad view character which is not taken into consideration to an atom level, and the file 2 is performed.

[0351]Such a system can start and use a corresponding point from a program of a practical semiconductor manufacturing system of drawing 1. After realizing and putting a process simulator of only such calculation in practical use on a computer conversely, it is also possible to perform combination with a actual process unit. Namely, a semiconductor manufacturing system of drawing 1 can be built from a system of process unit V, spectrum meter VI, and Drawing 131, An external output terminal of spectrum meter VI is connected to a communication port of the computer 1 using the suitable cable 19, and comparison processing of an actual measurement and a calculated value is performed. The result is sent to the control means 23 of a process unit similarly connected to a communication port of the computer 1 using the suitable cable 21, and is reflected in a process control in real time.

[0352]About process induction stress, such as oxidation and silicide, a two-dimensional simulator has already reached even a utilization level mostly. However, this artificer discovered that a three dimension is indispensable for a design of a fine element, and completed this invention as a three-dimensional simulation so that it might explain below.

[0353]In an old simulation, even if it uses oxidation and uses diffusion, a place of a join office belongs to a diffusion method rule of Fick. ** which that a substance does not move but situations differ greatly divides in a two-dimensional problem treating a x-y side when it is good noting that there is no movement of a substance in the direction of z which is the 3rd axis, but it is "stress." ****** and SHIRISAI Dison of this are the same as that of oxidation.

[0354]Namely, stress calculation in two dimensions of TSUPEM4 said to progress most in the actual condition set stress to sigma, set displacement to v, viscosity was set to mu, and it set a BOASON ratio to nu, and was based on the following formulas.

[0355]

[Equation 134]

sigmaxx+sigmayy=mu/(0.5-nu) - (**v$_{XNO}$**x+**vy/**y)

sigma xx-sigma yy = 2micro- (**vx $_{NO}$ **x-**vy/**y)

sigmaxy = 2micro- (**vy$_{NO}$**x+**vx/**y)

Understanding now is the handling of two-dimensional simple xy side, and it is that z ingredient has not appeared here. Although it is not visible explicitly here, Young's modulus E is treated as scalar quantity.

[0356]This artificer performed creation of a strict three-dimensional rigid matrix, and preliminary calculations of a strict plane direction operator. When only the result was described, in Si system, it turned out that it is as follows. namely[Equation 135]

**** of sufficiently thick two-dimensional plane strain (plane strain) is first considered to a depth direction using this formula. That is, about the case of (epsilonx!=O, epsilony!=O, epsilonz=O, epsilonyz=O, epsilonzx=O, epsilonxy!=O), when it substitutes for the above-mentioned formula, that of ****** understands the paragraph of sigmaz. Namely, sigma z=Cxz-epsilon x+ Cxz-epsilon y+ Czi-epsilon xy. The value of sigmaz also traced that it was never slight quantity. Therefore, the first ** for that the paragraph of sigmaz which the three dimension is indispensable and should be taken into

consideration also by two dimensions in the above-mentioned TSUPEM4 is missing to divide. Also in ******, it became clear at least in two dimensions that z ingredient of the 3rd axis also comes out in the case of the stress of oxidation or silicide.

[0357]Next, the above-mentioned formula was transformed and rigid-matrix Cij in each actual field was calculated. The elastic matrix of single crystal Si is described first.

[0358]

[Equation 136]

Come out, and it is and is C11=1. 7 They are 2**15Gpa, C22=66**6GPa, and C44=-82**9GPa. Understanding now is never single scalar quantity. This is made to operate a field rotational operator, and it is as follows when it asks about the section (110) of the often seen [first usually] silicon crystal (refer to Drawing 132 (B)).

[0359]

[Equation 137]

What is understood now is understood that contribution of z ingredient is very large. About the field top which becomes a problem by bipolar ** (111), it is as follows (refer to Drawing 132 (B)).

[0360]

[Equation 138]

Although such converting operation was indispensable, in the old simulation, it was not taken into consideration but it became clear that the accuracy of the analysis of the fine structure is low. So, in this invention, a three dimension will be dealt with like the above. This is another aspect of this invention.

[0361]

[Embodiment of the Invention]Hereafter, various working example of this invention is described.

[0362]working example 1 -- this working example starts directly the prediction function of the optical spectrum which is one of the big features of this invention. It describes in detail once again here from the technique which this invention persons invented.

[0363]First, a few is described from the conventional technical level about the art about a high reliability-ized oxide film design, its evaluation pertinent art, etc. As a publicly known publication, there is "ThePhysics and Technology of Amorphous SiO_2" Plenum Publishing Corporation and ISBN 0-306-42929-2, for example. In this publication, the result of IR and the result of Raman are indicated as an optical measurement result of various oxide films. This publication is called thing outstanding especially as an argument of an atom level.

[0364]It is argued by p.63 of this publication by pole MAKUMIRIAN (Paul McMillan) how the Raman signal of an amorphous oxide film changes with processes. Drawing 71 and drawing 72 are the results of being measured by pole MAKUMIRIAN. For example, the curve a of drawing 71 shows the Raman measurement result of the usual oxide film, and the curve b shows the Raman measurement result of the densified oxide film.

[0365]In the former, these both spectra should be compared, for example, moisture should **** by densifying, and the spectrum should change with these. Drawing 72 sees a spectrum before and after carrying out pressure impression for single crystal crystal. It is supposed that the place of 610 and 500 cm−1 has change especially. However, it glances first, and the variation of a spectrum is very small and art is required very much about where its attention should be paid and whether it should be regarded as a capable difference so that it may understand now. A still more complicated experience is required for identifying the variation of a substance from the amount of spectral changes.

[0366]Since it is in such a situation, in development of a new material which will be further needed from now on, there is a thing without the identification table of a spectrum plentifully, and the interpretation of a spectrum becomes a serious obstacle.

[0367]From p.71 of the above-mentioned publication, Hitoshi Kobayashi is seeing change of the Raman spectrum of the oxide fiber under high stress. A part of the result is shown in drawing 73. Here, the case where the case that stress is not impressed, and 3.5% of hauling strain are impressed is shown to the SiO_2 fiber. When 3.5% of hauling distortion is added so that drawing 73 may show, the place near the 450 cm^{-1} has change. However, the variation of a spectrum is very small and art is required very much about where its attention should be paid too and whether it should be regarded as a capable difference

so that it may understand also here. For identifying the variation of a substance from the variation of the spectrum, experience is required further.

[0368]In the above-mentioned publication, Kobayashi has tried the interpretation of the spectrum using drawing 74. If a hauling strain is received so that drawing 74 may show, it is supposed that the tetrahedron portion of 109 or 5 times of SiO_2 structure will be distorted. However, he has only carried out only 1 set of tetrahedron structures, and is not arguing about what kind of relation it is as the next tetrahedron portion at all. Actually, since it is a certain limited temperature, it should certainly be accompanied by distribution of the angle.

[0369]If quantitive distribution is not grasped as this invention person described on these Descriptions repeatedly, it will become about far from the analysis of a spectrum. The argument same as drawing 33 is developed by Kobayashi. Drawing 33 (a) is SiO4 as a function of an O-Si-O bond angle. It is a characteristic figure showing the wavelength of normal mode vibration of a tetrahedron. Drawing 33 (b) and (c) is a characteristic figure by the decoupling in the V4 mode produced by stress showing reduction in strong.

[0370]Drawing 76 is a defect model figure in the oxide film by W.B.Fowler indicated to p.107 of the above-mentioned publication. (a) of drawing 76 shows some coupled models of completeness alpha type Quartz, and are long combination and S of the inside L of a figure is short combination. (b) shows the model based on E1', (c) shows an E4'model, and (d) shows an E2'model, respectively. (b) The unpaired electron in − (d) is expressed with e−.

[0371]drawing 76 also shows −− as −− the above-mentioned publication −− the tetrahedron structure of 109.5 degrees −− two pieces −− or one piece is prepared and it is arguing about deficit structure. However, as mentioned above, it should certainly be actually accompanied by distribution of the angle at a certain limited temperature. Therefore, if calculation of a certain kind of many is not performed, it is far from the analysis of a spectrum about.

[0372]Drawing 77 is an example of execution by the new molecular dynamics simulator which this invention person etc. created. Si used 32 pieces and oxygen used 64 pieces. There were 520 reciprocal-lattice points. A vertical axis shows the rate of change of volume, and a horizontal axis shows time, respectively. Becoming the external pressure and a balance mostly after [of drawing 77] 1000 ft was confirmed. For example, the O-Si-O angle, the Si-O-Si angle, and O-Si distance at this time are shown in drawing 24.

[0373]The huge data equivalent to the "family register" of each atom is required so that drawing 24 may show. This invention persons are preparing some devices also for the calculation technique. For example, what is necessary is to sometimes extract the mode of vibration with which the selection principle of infrared absorption is filled from the time series data of the vibrational motion of the atom of ****, and just to ask for the frequency in infrared absorption. Anyway, such a trial does not still have an announcement and this can be said to be new "arms" of process development.

[0374]Using a molecular dynamics system, enough, this invention persons set time as 0, and make even time t sampling time now after that in the place which reached the balance. Time correlation was searched for as follows. that is, it comes out. M (t) is polarizability and is expressed with a following formula here. Integral value of the above-mentioned formula − It is the value with which it integrated from infinity to infinity.

[0375]

M (t) =sigmae$_i$−r (t) −− (1362)

⟨M(t) −M (0)⟩ expresses the autocorrelation function of M.

[0376]ei is a charge number in the point here, and i is a number of particles. Although r is a vector and the measurement starting point does not have restrictions in particular, it is good to take on the square of calculation cells.

[0377]What is necessary is just to ask for s (t1), s (t2), s (t3), s (t4), s (t5), s (t6), s (t7), and s (t8) in each time, in order to search for time correlation.

[0378]for example, it crosses to the whole sampling time −− sometimes −− the calculated value of the coordinates position of ****, and its kinetic energy −− quantity of motion etc. exist over all the particles further. And distance, those angular-position relations, etc. between still more nearly mutual particles are calculated.

[0379]This invention persons calculated also about some crystalline oxide films and an amorphous oxide film. A part of the result is shown in drawing 78. That is, drawing 78 shows the calculation result of the Si-O distance of single crystal cristobalite as one example. Drawing 79 shows the calculation result of a Si-O-Si angle in case there is a deficit. Drawing 79 shows around a deficit that movement is confused greatly. It also performed changing various concentration of these deficits and asking for the same action.

[0380]Drawing 80 is an example of execution of the new molecular dynamics which this invention person etc. created, and simulates a motion of an atom. A large ball shows oxygen among a figure and the small ball shows Si. (a) of drawing 80 shows the atom in XYZ space, and (b) shows the projection to the XY side. Although it was not able to be shown to that locus here, in this example of a single crystal, the atom also mainly understood that the atom was exercising preferentially in the direction of the median line of XY axis. $M(t) = sigmae_i - r(t)$ which this showed in the above-mentioned formula -- (1371)

A big bias will be shown in ****** and a spectrum peculiar to a single crystal will be shown as a result.

[0381]This invention persons changed measurement temperature and performed the simulation also with the situation of the action of an individual atom, and the natural frequency based on this, and the case where distortion is added further. Drawing 81 and drawing 82 show those examples. That is, drawing 81 is a figure showing a stress prediction result with same X-ray-spectrum prediction figure by the new molecular dynamics simulator by this invention and drawing 82.

[0382]Two working example artificers enabled it to also perform prediction of the spectrum of an oxide film in case there is an oxygen deficiency, and enabled contrast with a actual oxide film. The example made computable to the optical property of an oxygen-deficiency oxide film as working example 2 is shown.

[0383]When an ab-initio molecular dynamics method is used, it does not become a problem, but in the case of the molecular dynamics method which uses TTAT potential and BKS potential, when treating an oxygen deficiency, it becomes with a problem how best sets up charge of each atom. This is because combination is extended, or Si-Si combination arises and it becomes impossible to assume a fixed electric charge, when distortion becomes large dramatically. For example, if distribution of an electric charge changes actually and polarization becomes large by the elongation of Si-O combination, it will be expected that the electrostatic energy of stretching vibration becomes large and the peak pitch of IR becomes large.

[0384]Then, the balanced electric charge approximation (Charge equiliburation approach) using the ionization potential and the electroaffinity in which this invention persons had been tried by Rappe-Goddard for alkali and hydrogen, It applied to SiO_2 for the first time, and electrostatic potential was calculated by having incorporated amendment of the electric charge, and the technique of calculating movement and IR of each atom was performed.

[0385]They are treated with balanced electric charge approximation, assuming the electrostatic energies of a system to be the ionization energy of each atom, an electroaffinity of each atomic pair, and a function of each atomic charge, It is the technique of solving a number equivalent to an atomic number of simultaneous equations, and asking for each atomic charge from conditions that the atomization study potential of each atom is equal, in an equilibrium situation.

[0386]IR line spectrum and the conventional example at the time of using this method for beta-quartz were shown in drawing 83. By using this method, peak frequency shifted to the low frequency side about ten percent. This value is in agreement in survey and better accuracy. When $a-SiO_2$ also used this method, structure and an IR spectrum are enabled much more to relate with high degree of accuracy, and contrast with survey could be performed effectively.

[0387]The key map showed intelligibly the method which this invention person etc. invented to drawing 84. The search technique was shown in drawing 85.

[0388]This invention is not limited to above-mentioned working example. Especially other devices, such as a liquid phase device and a superconducting device, are effectively applicable to manufacturing by a clustering manufacturing installation. In addition, it changes variously in the range which does not deviate from the gist of this invention, and is feasible.

[0389]working example 3 -- here, the details about the direct prediction function of an optical spectrum

are shown as the 3rd working example. It creates on the computer of a-SiO_2 (amorphous SiO_2) first, and how to predict the optical spectrum is shown. a-SiO_2 was created by quenching, after fusing single crystal SiO_2 on a computer. Drawing 86 shows the temperature setting in the case of creation of a-SiO_2. Although it may carry out slowly, melting skyrocketed temperature here and melting was carried out rapidly. Then, the temperature was lowered with the comparable temperature falling speed. Drawing 87 is change of the pressure in that case, and drawing 88 is a volume change of a calculation area. In this process, this invention persons found out that the treatment of the external pressure and volume was important, when an experiential molecular dynamics method was used, or when an ab-initio molecular dynamics method was used and temperature was greatly fluctuated by rising and falling temperature. for example, in this example, if the external pressure is treated as a function of temperature so that volume may be maintained at about 1 law and a phase transformation may happen, and temperature rises, it will have set up so that a pressure may become large. The situation is shown in drawing 87 and 55.

[0390]However, when attention is not paid to volume at all but the external pressure is kept constant, large expansion of volume as shown in drawing 89 arises, and it completely becomes actual elevated-temperature melting SiO_2 with SiO_2 of low density remarkably in things. Also by a cooling process, it is, even if it goes into solid phase, and SiO_2 of colander low density is formed from ****. Of course, when potential energy was investigated, it was dramatically high, and it was in the unstable state. If it becomes like this, the contrast with survey will be difficult. Therefore, paying attention enough to the external pressure and creating a-SiO_2 found out the desirable thing here, and it performed it.

[0391]Change of the potential energy at the time of melting was shown in drawing 90. Since attention is paid to the external pressure, potential is rising gently, though it vibrates. Potential energy decreases gently in a similar manner also in the case of quenching. The temporal change of two sides of the field vertical to the cell c axis of the calculation area at this time was described in drawing 91. Since the technique of Parinello-Rahman is used for a cell so that shape may be changed according to a phase transformation, it is changing with melting.

[0392]Since quartz is a rhombus at first, the angle of two sides to make is 60 degrees. However, since a crystal structure will break and internal pressure will be uniformly applied each neighborhood as for it if it fuses, the angle of two sides to make is approaching 90 degrees. It seemed that it did not return to quartz even if quenched, but a rectangular parallelepiped was maintained at about 90 degrees.

[0393]When this invention persons created a-SiO_2, they found out that there was a point which it should be careful of one more point. It is related with the potential of Si and O. Also by ab-initio or the molecular dynamics method of experiential potential (ATTA potential or BKS potential), in treating a SiO_2 system, In order change of the potential energy by change of atomic arrangement is dramatically large, therefore to treat atomic movement, I hear that it is necessary to ask for atomic movement with high precision than the algorithm of the usual Velret, and it is.

[0394]Drawing 92 shows change of the potential energy at the time of asking for atomic movement with the algorithm of the usual Verlet, change of kinetic energy, and the sum of both energies. Total calories should become fixed when there is no exchange of energy with the external world. However, in the algorithm of the usual Verlet, since integration of the equation of motion drawn from raglan JAN is not performed in sufficient accuracy, a conservation of energy is not performed in this way. In order to raise integration accuracy, the situation did not change small the time interval which is an integration interval mostly at all. When this investigated, it turned out that it is peculiar to the material resulting from the potential of oxygen being dramatically steep.

[0395]then -- improving the algorithm of Verlet, in order to treat oxygen correctly -- the time -- ****** -- it asked until the individual atom of the acceleration of movement was high order, and it integrated with this, and saw in quest of speed and a position. Then, as shown in drawing 93, kinetic energy is changed by potential energy and an opposite phase, and total calories came to be kept constant. the exact treatment of such energy should do -- when there was nothing, according to the result which this invention persons performed, at an elevated temperature, the badness of calculation

precision broke in the case where atomic movement is intense, liquid SiO_2, etc., structure broke disorderly by the cause, and creation of a−SiO_2 was not completed. The IR spectrum has also completely differed from survey.

[0396]As mentioned above, this invention persons made it possible to create a−SiO_2 on a computer for the first time by elaborating uniquely in creation of a−SiO_2. Thus, created a−SiO_2 had a little long Si−O bond length as compared with quartz, and, moreover, Si−O length had fallen within the fixed range. In melting SiO_2, although Si−O of bond length smaller than the Si−O length in quartz existed mostly, when it cooled, this of Si−O length was lost, and he became only a combination longer than quartz. When the coordination number was counted and the first contiguity was set to 2A, 4 coordination was most, and 3 and 5 were mixed for a while and they did not produce Si other than it. 2 coordination of oxygen was almost the case.

[0397]Next, temperature was kept at 900 ** and structural relaxation of the time for 2 nanoseconds and the SiO_2 was carried out until potential energy reached a balance, in order to apply hydrostatic pressure or optically uniaxial stress to a−SiO_2 and to carry out prediction computation of the structural change of a−SiO_2 according to various stress fields. The structure of done various a−SiO_2 was changed into numerical values, such as each, an atom position, speed, acceleration, its primary differential value, a cell fundamental vector, and cell fundamental vector displacement speed, and was saved, respectively.

[0398]After carrying out so far and creating various a−SiO_2 structures, it asked for the IR spectrum from each. It asked for the IR spectrum from the dipole moment. The dipole moments M are following formula M=sigma qi and ri. −− (1461)

************* is made. Here, qi is an electric charge of the atom i and ri is a position. When searching for this position and a system is neutral (sigmaqi =0), the value of a dipole moment becomes the same for anywhere about the starting point r0. It, [Equation 139]

r0 =sigmaqi, M=sigma qi =(ri −r0) sigmaqi and ri−sigma qi, and ri −r0 sigma qi=sigma qi, and ri −− (1462)

It is because it becomes. Since a paragraph which r0 requires remains when a system is non−neutrality, an absolute value of a dipole moment changes with how to take the starting point, but when the Fourier transform is carried out, it turns out that frequency only appears in an ingredient of zero and does not influence others. In asking for this dipole moment, this invention persons have noticed that one−point cautions are required for how to take the atom position r. Since a periodic boundary condition is used for it when a molecular dynamics method is used for it, it is losing a discontinuous change of a dipole moment resulting from an atom left in − x direction of a cell entering from + x direction.

[0399]In consideration of being only carrying out a thermal oscillation and a−SiO_2 not being spread so greatly in temperature which actually measures IR, r used in the case of dipole moment calculation, Even if a periodic boundary condition was not considered but it went away from a cell in − x direction, a moment was calculated by having treated, when the position besides a cell had an electric charge. That is, it decided to deal with both of two atom positions, an atom position in consideration of a periodic boundary condition, and an atom position which does not take a periodic boundary condition into consideration, in the case of individual atom movement calculation. Thus, an example of a temporal change of a dipole moment for which it asked was shown in drawing 94. Since it was three−dimensional calculation, a dipole moment for x, y, and z all directions was obtained.

[0400]In order to ask for an IR spectrum, as the first step, the Fourier transform of this dipole moment is carried out, and it asks for a power spectrum which is IR line spectrum. The example was shown in drawing 95. A peak position of an IR spectrum can be predicted in this stage. That is, it is that a big peak appears in about 1000 cm^{-1}, and that a big peak appears in about 500 cm^{-1}. This result was in agreement with IR survey of a−SiO_2.

[0401]In order to ask for an IR spectrum, this line spectrum I (omega) is multiplied by a function of omega and the temperature T, and it asks by the following formula.

[0402]

[Equation 140]

= [alpha (omega)] (4pi 2/3hcn) and omega-(1-exp (-h omega/kT)) -I (omega)
-- (1463)

By calculating IR of a-SiO$_2$ in various stress fields, a stress field, the structure of a-SiO$_2$, and the details (a peak shift, peak show RUDA, etc.) of the IR spectrum were associated. Thereby, contrast with survey was attained.

[0403]The molecular dynamics simulator which this invention persons developed newly is applied to drawing 96 here at alpha-SiO $_2$, The calculated IR spectrum is shown, the molecular dynamics simulator which this invention persons developed newly to drawing 65 is applied to a-SiO$_2$, and the IR spectrum as which it was predicted when the external pressure was added is shown. The computational procedure by this invention persons is shown in drawing 100 and Drawing 101. A in the formula of movement of each atom within the block B in drawing 100 and B are paragraphs shown in a following formula.

[0404]By using a system concerning working example 4 this invention, phenomena, such as a substrate and plastic deformation of an interlayer film, can be foreknown by a size of induction stress in process, prediction of the ingredient, and also the grasp of detailed relation with the stress and material physical properties. A stress problem is mentioned as an example especially in this working example. It was examined whether the reduction would be aimed at, having predicted stress induction how and taking a process variation range into consideration.

[0405]It is indispensable to a fine element process design of these days to take into consideration stress at the time of process advance. About stress, the following phenomena arise, for example.

[0406](1) In an embedding isolation method, trench a Si substrate and embed SiO$_2$ here. In this case, by the difference of a coefficient of thermal expansion between a Si substrate and SiO$_2$, distortion and stress may remain and a crystal defect may be induced depending on a heat history. Therefore, it is necessary to draw up element structure and a manufacturing process which can reduce remaining stress as much as possible.

[0407](2) It is becoming frequent to use a Si substrate with low interstitial oxygen concentration from the purpose of creating a quality oxide film. In such a situation, Si-substrate intensity decreases and it is easy to induce plastic deformation.

[0408](3) For the purpose of formation maintenance of a shallow joining layer, and maintenance of a well area, it has increased as for a burden like heat processes, such as annealing and an oxidation process, in a substrate further by adoption of RTP.

[0409]In such a situation, with how generating of a defect is deterred. If a value with larger stress than default value and its change predicted value is observed in the middle of a process, while clarifying the cause immediately, monitoring, in a future process, it is important that it is shown how correction should be added. This is much more important in a clustering tool.

[0410]A kind of stress and identification are very important further again. It is also important to also pursue principal stress and the principal surface of the maximum stress and to pay one's attention to decomposition shearing stress, although it is important. For example, when Si (100) board is used, the sliding surface of the highest priority is a field as shown in Drawing 102 (111). Although the [100] directions are slip directions on this (111) field, it is thought that a time of shearing force working is the most dangerous in this direction.

[0411]An output of these identifications is also possible for a simulation system by this invention persons. Thus, oxidation of a trench portion is first taken up for cautions with a purification to plastic deformation here, and a design manual for obtaining the shape of the oxidizing form, and stress distribution and further predetermined shape is described. For example, although it is said that stress has contributed "sharpening" and a "more round" phenomenon of oxidation of a trench angle, the actual condition is that the structure is not known yet.

[0412]While understanding these phenomena in detail, it is required first to advance an exact process design which suppresses the above "sharpen" and advances "it is round." If induction stress is not grasped exactly, oxide film shape cannot be grasped correctly, either. a problem of stress is only a problem of plastic deformation -- they are also not **** but shape grasp, and an item further indispensable also to impurity distribution grasp under a stress field. Although prediction of oxide film thicknesses after a LOCOS process of a SOI substrate which will be developed with an element after

1G of future is divided for the time of oxidation advance unlike the usual Si substrate and it is easy to be influenced by stress, the quantitative prediction is a more complicated problem.

[0413]In such a background, work must be extended instead of the conventional oxidation diffusion model even to action grasp of an oxidizer under stress, and an understanding of an oxidation phenomenon under stress and impurity re-diffusion under stress. And it must be calculated at high speed for a short time. This invention persons created generating and prediction of redistribution of stress, and the still more nearly computable new high-speed general-purpose process simulator portion to a part for a point defect two-dimensional diffused part under stress, and added this to an atom level simulator. That is, the high-speed two-dimensional oxidation / diffusion / stress / modification process simulator part by original development were added to a parent of an atom level materials design system.

[0414]Survey of in situ observation of stress used micro Raman and FT-IR. A calibration of these measuring instruments was performed beforehand. When an operation sheet is inputted, Si and the amount of many [physical-properties] about SiO_2 are beforehand performed immediately by an atom level materials design system, and are calculated. This is sent to high-speed two-dimensional oxidation / diffusion / stress / modification process simulator part.

[0415]This invention persons first describe phenomenon analysis of "sharpening" and "more round" oxidation traced using this new high-speed two-dimensional oxidation / diffusion / stress / modification process simulator part, and show a basic examining result of an embedding isolation process, etc. as an example of application further. Cubical expansion will be caused, if Si oxidizes and it becomes SiO_2. Although there is viscoelasticity in SiO_2 and a part of that stress is eased at this time, stress still remains to both Si and SiO_2.

[0416]Oxidation of a trench corner is taken for an example, such a situation is investigated, and what was illustrated is Drawing 103. First, at this time, although an oxidizer of the concentration C reaches SiO_2 and invades and goes into a SiO_2 film, also when [at which diffusion D' of an oxidizer is influenced by the stress sigma in a SiO_2 film] it is a Si/SiO_2 interface and an oxidizer reacts to Si further, it is influenced by remains accumulation stress in a substrate.

[0417]As a concrete effect, when the compression stress sigma exists in SiO_2, a network atomic interval will control diffusion of narrowing and an oxidizer, for example. When the compression stress sigma is accumulated on a field of a Si substrate, Si atom interval will suppress invasion of narrowing and an oxidizer, and will stop an oxidation rate as a result also here.

[0418]If an ingredient of a x direction of the principal stress S is set to sigmaxx and an ingredient of a y direction is set to sigmayy now, about stress on a two-dimensional side, a following formula (1531) and an expression of relations - (1534) will be materialized. mu is coefficient of viscosity, nu is a Poisson's ratio here, and u is displacement.

[0419]

[Equation 141]

By the way, generally the temperature dependence of the coefficient of viscosity mu can be expressed by the above-mentioned formula (1534). Here, VISC.O and VISC.E show a proportionality constant and activation energy, respectively. Therefore, when the above-mentioned angle stress type is seasoned with the temperature dependence of mu, it turns out that the ingredient of each principal stress decreases with a rise in heat. Reaction constant kappas ' in case the oxidizer which reached even the Si/SiO_2 interface reacts in a Si surface can be similarly expressed in writing like the above-mentioned formula (56). It is a value in case, as for kappas, stress does not exist here. Here, sigman is sigman =- (sigmaxxnx 2+sigmayyny 2+2sigmaxynx ny), and is sigmatau=- (sigmaxxny 2+sigmayynx 2-2sigmaxynx ny). VR is a parameter. This formula shows that an oxidation reaction constant decreases, while compression stress increases. The influence of the remains accumulation stress in a substrate in case an oxidizer reacts to Si by the above-mentioned Si/SiO_2 interface is this.

[0420]Diffusion coefficient D' of an oxidizer in an oxide film can be expressed by the above-mentioned formula (1531). p is expressed by following formula here. That is, it is p=-1 / 2 (sigma xx+sigma yy). D is a diffusion coefficient in case stress does not exist. Implications of this formula can be interpreted as

follows. That is, stress sigmaxx and sigmayy take hauling to positive, and have taken compression to negative. Therefore, compression stress exists in a film, and if a substance is in a dense state, it is shown that a diffusion coefficient becomes small. The above-mentioned formula expresses this.

[0421]A computational procedure of only this portion which this invention persons found out is shown in Drawing 104. First, it asks for concentration of an oxidizer in each node in a Si/SiO_2 interface. After an appropriate time, a temporary oxidation rate in each 1st node is computed based on this concentration. Moreover, the amount of growth u of a SiO_2 film in each node is calculated. It asks for the stress S from the above-mentioned formula (57) using this u. using this stress -- a formula (56) and a formula (1531) -- an oxidation rate is further recalculated again using a formula (1534). And again, an amount of growth is calculated and stress is computed. And if enough completed by stress, advance of new oxidation time will be begun anew. That is, a Newton's method is used.

[0422]As shown also in this Drawing 104, stress calculation at the time of oxidation requires very prolonged calculation time. By typical trench structure, 900 ** oxidation was tried by 1300 initial nodes. An oxidizing atmosphere was made into 100% of dry oxygen, and oxidation time was made into 300 minutes. Computation time was investigated using EWS Sun4. If it is conventional technology, time for 15900 minutes will be required in general. This reaches also in about ten days and it is very unsuitable for practical use as [this].

[0423]About calculation of a Newton's method portion, this invention persons introduce a ** part principle, save the last converging state, and advanced convergence calculation using primary differentiation of this. By this method, 900 ** - 1100 ** were able to be taken for an example, and conventional method is short to 1/1000 or less, and it was able to carry out. Thereby, this simulator advanced rationalization of a material property value, and improvement in the speed of operation part, and reached till a place which can be used as a tool for real time. This invention persons investigated accuracy of a time dependency value of oxide film thicknesses, the shape reproducibility of a trench corner, etc. as basic accuracy of a simulator further.

[0424]Drawings 105-77 summarize a result of having investigated temperature of growth thickness, and time dependency in a graph using the above-mentioned simulator. Although not displayed here, oxygen tension questioned this invention persons also about a decompression action at the time of 10% or 1 more%. As a result, since it goes on while stress accompanying expansion of an oxide film eases enough when an oxidation rate is slow, stress is not accumulated in a substrate, therefore a uniform oxide film is formed also in a convex portion. Oxygen tension was gradually understood that a method of mentioning and going is effective, dropping oxygen tension, making an oxidation rate late in early stages of a result of this invention persons' prudent examination, especially oxidation, and making it ease enough.

[0425]This invention persons investigated why "it is round" would occur, saying "sharpen" of a trench angle using this system. As already stated, it is necessary to take some elements into consideration in oxidation of a trench angle. Five backbone corresponding to the following is described.

[0426](1) Inside of these [Si-surface stress-dependency model this invention persons of the plane direction dependency model (5) oxidizer / Si reaction of a stress-dependency model (4) oxidation rate of oxide film visco-elastic model (2) silicon flexible model (3) oxidizing agent diffusion] five models, But a dominant thing traced that it was stress of a Si substrate of the 5th model, i.e., a Si/SiO_2 interface, also unexpectedly. Here, dry oxidation in 900 ** will be taken up. If shape of an oxide film at this time and shape of a Si/SiO_2 interface are often seen, shape "is sharpened" still will not almost be accepted. When it became after 300-minute progress by 900 ** dry oxidation, in oxidizing temperature of about 900 **, a phenomenon in which a trench angle sharpened was analyzed as follows.

[0427]That is, if it is till about 100 minutes, stress will not be generated so much. However, compression stress concentrates on the inside of a SiO_2 film of a corner, and the Si tip part side by SiO_2 cubical expansion with oxidation. At about 900 **, the viscous flow effect is small and a shape relaxation effect of an oxide film is especially small. And oxidation reaction is deterred by compression stress in a Si surface, and it sharpens as a result. however -- if it becomes 1100 ** -- the viscous flow effect -- **** -- a shape relaxation effect of an oxide film which it hears sets, and is -- ** And there is no accumulation of compression stress in a Si surface, and it becomes round as a result. Drawing 108

showed this situation. The predicted value of these stress was able to carry out the measurement check in less than **10% of accuracy as a result of the Raman measurement or IR measurement.

[0428]Preparing the above knowledge, this invention persons applied the above-mentioned simulation system to a part of basic examination of STI (Shallow TrenchIsolarion) for the purpose of area reduction of an isolation region further. Basic examination of a more round process of an upper corner of a trench was advanced especially here. Oxidizing temperature is 1100 **, oxygen tension is 3%, and it saw about the 100-minute progress back. As a result, the following things are understood.

[0429](1) In the beginning, oxidation of poly Si and a crevice between retreat parts of a buffer oxide film oxidize. At this time, a corner sharpens and is feeling.

[0430](2) Oxidation progresses succeedingly, a crevice oxidizes, if filled, supply of an oxidizer will decrease rapidly, oxidation from the side will become rate-limiting, and a corner will be roundish as a result. The neighborhood of a crevice of principal stress is large.

[0431]On the other hand, stress distribution at the time of oxidation by 50% of 1000 ** oxygen tension was examined. Time is after 30-minute progress. As a result, compared with stress distribution of previous 1100 ** oxidation, it turns out that stress is large a little. The above consideration shows that it is the first condition not to store up remaining stress in a Si surface, in order to deter **** of a trench corner. It can consider stopping an oxidation rate enough and making modification relaxation of an oxide film cause enough also at low temperature as a fundamental measure for this etc.

[0432]This invention persons advanced union-ization with a plastic deformation simulator further. As a result, it turned out that not only oxidation but modification after TEOS film deposition, etc. are investigated.

[0433]Based on the above result, especially this invention persons saw a value projected on a field (110) with a two-dimensional simulation system paying attention to decomposition shearing stress on a field which is a sliding surface (111). If heat unevenness occurred within a wafer 300 degrees as a heat history although what is necessary is just to have been a part for /, and even a part for /was reached 600 degrees selectively, it also traced with stress that a rearrangement occurred depending on a part.

[0434]The above reserve knowledge is prepared separately and this invention was applied to a manufacturing process of a bipolar CMOS in real time. That is, contrast, and the amount of dispersion and a permissible dose of serial prediction by a simulation and the minimum necessary in each process which are a factor of each process further, a spot measurand, were examined. An example carried out about oxidation time dispersion of sacrifice oxidation and permissible doses, such as shape, is shown below especially here.

[0435]A basic process is as being shown in Drawing 109. Furthermore it continues and there is each process of sacrifice oxidation -> of a RIE etching -> oxidation -> polycrystal Si embedding ->CMP-> polycrystal Si portion for isolation. A factor of each process has the range of fluctuation. In this working example, it is a portion of sacrifice oxidation of a polycrystal Si portion, especially its attention was paid to oxidation quantity. As the range of fluctuation of oxidation quantity, a real-time calculation result is shown about two, a case of oxidation quantity zero, and the specified quantity. Change of oxidation quantity, oxide film shape in a LOCOS process of continuing the shape of an oxidizing form of that way, stress distribution, and also next, and the ingredient characteristic of that stress is shown.

[0436]Drawing 110 a distribution map of 1000 ** and sigmaxx at the time of an end of a LOCOS process, and Drawing 111, Similarly a distribution map of 1000 ** and sigmayy at the time of an end of a LOCOS process, and Drawing 112, Similarly a distribution map of 1000 ** and sigmaxy at the time of an end of a LOCOS process and Drawing 113 a distribution map of sigmaxx when temperature is lowered to 25 ** after an end of a LOCOS process, and Drawing 114, Similarly a distribution map of sigmayy when temperature is lowered to 25 **, and Drawing 115 show a distribution map of sigmaxy when temperature is lowered to 25 ** after an end of a LOCOS process after an end of a LOCOS process, respectively.

[0437]As shown in these figures, when there is no sacrifice oxidation over a polycrystal silicon film, the surface of a polycrystal silicon film and the surface of a nitride have gathered after CMP. When a LOCOS process is performed in this state, an oxide film which expanded by oxidation will push from the side of a nitride. On the other hand, since a nitride bends and goes well when sacrifice oxidation is performed also with some, stress eases and goes. The result was shown in Drawing 116.

[0438]This invention persons use the above which this invention persons have advocated, and a

simulation system which made a high-speed molecular dynamics simulator using experiential interatomic potential, and a general-purpose process simulator unite, An oxidation process, an interlayer insulation film formation process, and after passing through a wiring process further, it traced that stress which remained to a Si substrate and an oxide film of a MOS device had big influence on the electrical property of an oxide film especially.

[0439]While this invention persons predicted a stress generation process and a generation part in real time one by one using the above-mentioned simulator, for example, what kind of holding property a tunnel oxide film of an EEPROM element portion shows eventually made them output. An element in a present progressive can predict so much what kind of the characteristic is given to allowable width of the holding property of an element obtained eventually by using this system. This is the effect of a system which becomes this invention. A process of continuing can be corrected or avoided so that a system of skillful Lycium chinense may be used and the optimal characteristic can be obtained during process progress. This working example is shown below.

[0440]working example 5 -- this working example shows an example which applied this invention to a stress problem in a silicon oxidizing film. A stress problem is important in order to control a crystal defect in inside of a silicon substrate, and generating of a rearrangement, but not only in it but various materials, it is important also as a factor which affects membraneous quality.

[0441]In a silicon oxidizing film, oxidation stress resulting from cubical expansion at the time of silicon oxidizing and heat stress produced by rising and falling temperature have arisen, and these have affected quality of an oxide film. That is, if it says with an atom level, stress may affect network structure of silicon oxide and may influence even the Tetrahedron structure which is unit structures of a SiO_2 system. Influence is also brought to electric insulation if it lengthens. Then, this invention persons advanced an oxidation process, controlling quality of an oxide film, preparing structure in an IR spectrum and an atom level in silicon oxide, and knowledge to an electrical property.

[0442]First, this invention persons investigated structure and an electrical property in an IR spectrum and an atom level of silicon oxide as a preceding paragraph story. As shown in Drawing 117, a silicon (100) board was prepared, an isolation process was performed, and an element region separated by isolation region was created. Next, a silicon substrate was introduced into an oxidation system, and as shown in Drawing 118, a gate oxidizing film was formed. At this time, oxidizing temperature was variously changed from 800 ** to 1100 **.

[0443]Substrate temperature was made to lower after forming silicon oxide of predetermined thickness. At this time, a temperature fall of substrate temperature was performed in two steps, as shown in Drawing 119. The 1st step is the process of lowering substrate temperature to 900 **, and made substrate temperature quench. The 2nd step is a process made to lower from 900 ** to a room temperature, and consideration in particular was not carried out to a temperature falling speed. When oxidizing temperature was set as 900 ** or less, the temperature was lowered only in the 2nd step.

[0444]It opted for setting out of this temperature fall condition from analysis of a viscous relaxation action of an oxide film separately. Generally, at an elevated temperature, an oxide film becomes soft and is said to become easy to ease stress by viscous flow. Then, this invention persons investigated a stress relaxation action by viscosity in detail. An example which investigated change of the characteristic of stress relaxation by a temperature falling speed was shown in Drawing 120 and Drawing 121. In this example, oxidizing temperature was 1000 **.

[0445]When it holds at 1000 **, respectively and quenches by 600 ** / min after Drawing 120 performed a typical oxidation process, it is the result of investigating the maximum of principal stress of a direction along the surface at the time of cooling slowly by 6 ** / min. Stress eased in about 1 minute, by quenching, viscous relaxation was slight and, a case of 1000 ** maintenance, and in the case of annealing, a result shown in Drawing 120 showed only being superimposed on heat stress, and that it was.

[0446]Drawing 121 is a figure which made a horizontal axis temperature and plotted a stress action in the same temperature fall process. Stress relaxation is remarkable, an action of a viscous body or a viscoelastic body was shown, and stress relaxation hardly happened below 950 **, but Drawing 121 showed that an oxide film showed an action of an elastic body in a not less than 950 ** temperature range.

[0447]If the two-step temperature fall performed by this example is used so that it may guess from such example computation, By passing a temperature range which viscous relaxation produces as much as possible for a short time, it becomes possible to suppress viscous relaxation and various heat stress produced from a difference of a coefficient of thermal expansion of a silicon substrate can be set to an oxide film by moreover changing various oxidizing temperature.

[0448]Thus, when a tensile stress of the direction of a substrate face directly under silicon oxide was measured from a section using a micro Raman spectrum using a created sample, it was checked that various heat stress has induced in a silicon substrate. This invention persons compared a calculation result illustrated to stress induction measured value and Drawing 122 in these substrates, and guessed a stress value induced in an oxide film. In performing these stress calculation, this invention persons used material and a process prediction simulation system which a molecular level to a general-purpose level which this invention persons built included. As a result, a relation shown in Drawing 123 between oxidizing temperature and compression stress in an oxide film was obtained. Drawing 123 shows that the maximum of compression stress in an oxide film increases linearly with a rise of oxidizing temperature.

[0449]An IR spectrum was measured to an oxide film which produced compression stress formed as mentioned above as next preparation. On the other hand, computer prediction of oxide film structure when this compression stress is added, and IR PEKUTORU was performed using a classic molecular dynamics method. Drawing 124 shows change of calculation IR PEKUTORU by existence of compression stress addition.

[0450]Drawing 125 shows the result of measuring a wave number shift by stress of a Si-O-Si asymmetric stretch peak from measured value of an IR spectrum. When an actual measurement was compared with a calculated value, signs that an appearance wave number of an asymmetric stretch peak of Si-O-Si shifts to the low wave number side rather than a case where he has no stress addition are obtained from a calculation IR spectrum with compression stress, and it turned out that an experiment and calculation are well in agreement. Then, amorphous structure and IR full spectrum at the time of adding stress variously were calculated and prepared.

[0451]Furthermore, relation of stress and an electrical property was investigated as next preparation. An oxide film which has produced the above-mentioned various compression stress was used as gate dielectric film, a gate electrode was deposited on it, and Qbd was measured. Deposition of GE 1 ****** is 900 ** or less in temperature, and is ****** about all the processes so that viscous relaxation of an oxide film may not arise. And correlation with oxide film structure and Qbd which were predicted from the above-mentioned molecular dynamics calculation was investigated.

[0452]Drawing 126 is the result of a Si-O atom interval of the first contiguity searching for correlation with the frequency of occurrence of combination and Qbd used as 1.8 A or more, after computing a radial distribution function of a Si-O atom of an oxide film in various stress fields. When the frequency of occurrence from which a Si-O atom interval has become more than 1.8A exceeded 5% from Drawing 126, it turned out that Qbd is decreasing notably and Si-zero-atom interval and an oxide film dielectric breakdown are related. The amounts of IR spectral shifts are about 15 cm^{-1} and intermediary ****.

[0453]Change of amorphous NEFUTO work structure when compression stress is added to an oxide film, (1) Since density of an oxide film increases, two kinds of anticipation of anticipation that the degree of Si-O-Si bond angle decreases have been made from anticipation that Si-0 bond length decreases in number, IR measurement of (2) thin-film oxidizing film, and main KAMODERU. However, it newly found out that a rate of combination which increased density of an oxide film did not lead to Si-O bond length's simple reduction, but bond length distribution spread rather, and was extended by a simulator which this invention persons developed uniquely as shown in Drawing 127 increased. In addition, it found out to correlation with Qbd.

[0454]About a Reason for physical with correlation of Qbd and a postponed Si-O combination, although this invention persons have not solved details yet, they guess − ** of the Reason as follows from a paper reported recently. A citation paper is "electron hole capture by local deformation and impurity in oxide film" p.101-104 reported by Mr. Kaneda with "a thin film and a surface physics subcommittee report of research, and formation, evaluation and reliability of ultra-thin silicon oxide." According to a place which Mr. Kaneda calculated using the molecular orbital method program GAUSSIAN "if there is extended Si-O-Si, capture of an electron hole to oxygen of the center will be induced. Since

localization of the captured electron hole is strongly carried out into oxygen, to an electron, it works as a trapping center. As a result, many of oxygen captures an electron and they return to the original state. However, Si-O combination which acquires several electron volts energy released by recombination of an electron and an electron hole, is extended and is weak is cut, and it jumps out to between lattices, for example, the part can generate a-like secondary defect like an oxygen deficiency. It is reported ".

[0455]According to this invention persons, combination extended by stress addition increases like this report, and it is expected that an oxygen-deficiency defect is formed. Although various structures can be considered to an oxygen-deficiency defect, in structure where Si atom of oxygen-deficiency both ends was pulled apart greatly, an electronic state is also conjectured to change a lot, to form level in a band gap or to change to electron distribution which produces electrical conduction. And the insulation of an oxide film is imagined to deteriorate.

[0456]Since an IR spectrum of an oxide film in inside of a stress field could be predicted and correlation with structure in an atom level and an electrical property was further acquired by making the above preparations, this invention persons tried "correction of a manufacturing process."

[0457]A Si wafer which progressed to a predetermined process was introduced into an oxide film forming device, and an oxide film of desired thickness was formed in 1050 ** and dry O_2 atmosphere which contains chloride 5%. A wafer was quenched to a room temperature after oxide film formation, and an IR spectrum of a formed oxide film was measured. From measured value, a Si-O asymmetric-stretching-vibration peak wave number of an IR spectrum was read, and when a shift amount from the wave number when stress has not arisen was calculated, a shift of 17 cm^{-1} was measured.

[0458]From this shift amount, it was predicted that compression stress of about 0.2 GPa(s) is induced by oxide film in an oxide film. This shift amount was measured with shift critical-value [of 15 cm] $^{-1}$. Like this heat process, since it was detected that it is over a critical value, a process was stopped. And stress relaxation by high temperature annealing was performed as correction of a manufacturing process.

[0459]In order to compare an effect of this example, a high temperature annealing process was not added to some wafers, but a process was passed as it is. Annealing time, annealing temperature, a temperature falling speed, etc. which are the parameters of high temperature annealing for stress correction were computed in consideration of analysis of relaxation time by viscous relaxation prepared beforehand, and a re-diffusion action of an impurity diffused layer already formed into a substrate. In this case, 1000 ** and annealing for 30 seconds were performed.

[0460]Since it was less than a critical value when an IR spectrum was measured again and a shift amount was computed after an end of annealing, a process was continued as it was. Qbd was measured by case where a process is corrected, and a case where it does not correct. As a result, in a case where it corrects, 45C/cm^2 and a case where it did not correct made 5 C/cm^2, and an effect of process correction by this invention was acquired clearly.

[0461]In a wafer which has another structure, gate oxide of desired thickness was formed in 950 ** dry O_2 atmosphere. When a wafer was quenched to a room temperature after oxide film formation and an IR spectrum of a formed oxide film was measured, a peak shift amount was 16 cm^{-1}. Since this was over a critical value, an addition of annealing for stress relaxation was required for it, but when re-diffusion of an impurity diffused layer was taken into consideration, a solution of a suitable annealing condition did not exist. Then, it judged that process continuation was impossible for this wafer, and a wafer was discarded.

[0462]

[Effect of the Invention]In the device, division single wafer processing, or the clustering manufacturing installation which it not only solves the problem of the monitoring facility in clustering, but manufactures semiconductor devices, such as MOSLSI, according to this invention as explained above, Even if the "spot" "spot" measured value of a limited quantity in each device is extended to the maximum and there is no test piece, it goes on, while a request corrects as a process. [of measured value and limited qualitative contents] According to this invention, fluctuation of (i) each process element, the check of whether to perform by diagnosing the superposition phenomenon of a gap of each element as the

sequence of a (ii) request, and discovery of a (iii) change factor are also possible. furthermore -- again -- the feature of this system -- change of a (iv) process -- mathematical, the point it enabled it to deal with statistically and efficiently, and (v) -- the point to which a new inference engine was made to add, and (vi) -- it is in the point which added a new opposite direction system.

[Translation done.]

Drawings are not displayable due to the volume of the data (more than 200 drawings).

DESCRIPTION OF DRAWINGS

[Brief Description of the Drawings]
[Drawing 1]The figure showing the whole system by this invention.
[Drawing 2]The figure showing that the inclination to each direction of a potential size serves as power of each direction.
[Drawing 3]The figure showing the new abinitio molecular dynamics simulation system used for this invention.
[Drawing 4]The figure showing the effect of starting an operation with the second atom (j) through the second (j) from the third atom (k) further with first atomic (i).
[Drawing 5]The figure making r the distance between particles and making theta a particle angle and in which showing the relation of the principal and accessory of these amounts of many.
[Drawing 6]The figure showing positioning by the conventional calculation technique and the Takashina round partial differential method of this invention.
[Drawing 7]The figure which explains cooperation with the process variation calculation unit I to be the molecular dynamics simulator II.
[Drawing 8]The figure which explains cooperation with the process variation calculation unit I to be the molecular dynamics simulator II.
[Drawing 9]The figure showing **** for an example of the input sequence of wide use 2 and a three-dimensional process simulator.
[Drawing 10]The figure showing **** for an example of the input sequence of wide use 2 and a three-dimensional process simulator.
[Drawing 11]The figure showing a part of binary tree by working example of this invention.
[Drawing 12]The mimetic diagram of the Coulomb interaction at the time of ionization is shown.
[Drawing 13]The mimetic diagram of the Coulomb interaction at the time of ionization is shown.
[Drawing 14]The mimetic diagram of the Coulomb interaction at the time of ionization is shown.
[Drawing 15]Easy atomic structure MODERU ** is shown.
[Drawing 16]An alkaline metal halide molecule is shown.
[Drawing 17]The table of the valence orbital index zeta is shown.
[Drawing 18]The electric charge which dispelled and searched for the matrix (3063) is shown.
[Drawing 19]The electric charge which dispelled and searched for the matrix (3063) is shown.
[Drawing 20]The electric charge which dispelled and searched for the matrix (3063) is shown.
[Drawing 21]The calculation result of Coulomb interaction J between Si-Si is shown.
[Drawing 22]The electric charge of O is in 2 s, and the calculation result of JAB at the time of modeling the state where Si is in 2 s or 3 s is shown.
[Drawing 23]What summarized the procedure of the newly developed above-mentioned electric charge numerical orientation method in the crystal system and the amorphous system is shown.
[Drawing 24]The O-Si-O angle which is an executed result of the molecular dynamics simulator by this invention, a Si-O-Si angle, and the data figure showing O-Si distance.
[Drawing 25]The figure showing each subroutine including the variations calculation in the conventional simulation system.

[Drawing 26]The figure showing the procedure of the variations calculation in the conventional simulation system.
[Drawing 27]The characteristic figure showing the converging state of the conventional process and a change process.
[Drawing 28]The data figure showing the accuracy of a variations.
[Drawing 29]The data figure showing the accuracy of a variations.
[Drawing 30]The data figure showing the accuracy of a variations.
[Drawing 31]The figure showing the conventional impurity distribution by a simulation system and its example of change.
[Drawing 32]The figure showing change and its execution combination of the process by the conventional simulation system.
[Drawing 33]The figure showing some trees of search of the inference engine by the conventional simulation system.
[Drawing 34]The figure of optimization of the perovskite by the new abinitioMD simulator which this invention persons developed, and Si system crystal.
[Drawing 35]The construct figure of the simulator by original development by this invention person etc.
[Drawing 36]The flow chart of the simulator by original development by this invention person etc.
[Drawing 37]The figure of the example for C4v of the PTO perovskite by the simulator which this invention person etc. developed.
[Drawing 38]The lineblock diagram of perovskite $BaTiO_3$ and $PbTiO_3$.

[Drawing 39]The potential output figure of the perovskite PTO by the simulator which this invention person etc. created newly.
[Drawing 40]The example of creation of SiO_2 in the simulator which developed this invention person etc.

[Drawing 41]The output figure of charge of the perovskite PTO by the simulator which this invention person etc. created newly.
[Drawing 42]The example of distortion of the perovskite PTO by the abinitio/MD simulator which this invention person etc. created newly.
[Drawing 43]The example of the oxygen deficiency of the perovskite PTO by the abinitio/MD simulator which this invention person etc. created newly.
[Drawing 44]The example of movement of Pb of the perovskite PTO by the abinitio/MD simulator which this invention person etc. created newly.
[Drawing 45]The example of movement of Pb of the perovskite PTO by the abinitio/MD simulator which this invention person etc. created newly.
[Drawing 46]Some data of the simulator which this invention persons created
[Drawing 47]The figure of saw YATAUWA.
[Drawing 48]The figure of working example of this invention.
[Drawing 49]The key map showing how the in-situ monitor measuring device is added in the clustering tool used for this invention.
[Drawing 50]The figure showing signs that the method of making the limited measurand and sufficient information acquired from another side calculation contrasting is displayed as a picture [graphics / on a monitor].
[Drawing 51]The figure showing the temperature sequence as an example of the input data to the abinitio molecular dynamics simulation system by this invention.
[Drawing 52]The key map showing execution prediction of the atom level by the abinitio molecular dynamics simulation system by this invention.
[Drawing 53]The key map which visualized the atom level execution prediction by the abinitio molecular dynamics simulation system by this invention.
[Drawing 54]The figure showing aging of the Si-O-Si angle which is an example of execution about SiO_2 by the abinitio molecular dynamics simulation system by this invention.
[Drawing 55]The prediction figure of measured value change of the temperature which is the example output to the input sequence of drawing 51.
[Drawing 56]The distribution map of the coordination angle in membrane formation Si which is an

example of atom level execution by the simulation system by this invention.

[Drawing 57]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 58]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 59]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 60]The distribution map of Si coordination angle which is an example of atom level execution by the simulation system by this invention.

[Drawing 61]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 62]The example of atom level execution by the simulation system by this invention. The distribution map of the distance between Si-Si.

[Drawing 63]The distribution map of Si coordination angle which is an example of atom level execution by the simulation system by this invention.

[Drawing 64]The distribution map of Si coordination angle which is an example of atom level execution by the simulation system by this invention.

[Drawing 65]The distribution map of Si coordination angle which is an example of atom level execution by the simulation system by this invention.

[Drawing 66]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 67]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 68]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 69]The distribution map of the distance between Si-Si which is an example of atom level execution by the simulation system by this invention.

[Drawing 70]The figure showing the another whole system constituted by this invention.

[Drawing 71]The characteristic figure showing the conventional Raman measurement result.

[Drawing 72]The characteristic figure showing the conventional Raman measurement result.

[Drawing 73]The characteristic figure showing the conventional Raman measurement result.

[Drawing 74]The figure showing the model for explaining the conventional Raman measurement result.

[Drawing 75]The characteristic figure showing the strength reduction produced by the characteristic figure and stress which show the wavelength of normal mode vibration of the SiO_4 tetrahedron as a function of an O-Si-O bond angle.

[Drawing 76]The model figure showing the defect in SiO_2.

[Drawing 77]The characteristic figure showing the example of execution of the molecular dynamics simulator by this invention.

[Drawing 78]The characteristic figure showing the example of execution of the molecular dynamics simulator by this invention.

[Drawing 79]The characteristic figure showing the example of execution of the molecular dynamics simulator by this invention.

[Drawing 80]The figure showing a motion of the atom which is an example of execution of the molecular dynamics simulator by this invention.

[Drawing 81]The characteristic figure showing the X-ray-spectrum prediction result which is an example of execution of the molecular dynamics simulator by this invention.

[Drawing 82]The characteristic figure showing the stress prediction result which is an example of execution of the molecular dynamics simulator by this invention.

[Drawing 83]The characteristic figure showing the computed result by the molecular dynamics simulator which this invention persons developed newly.

[Drawing 84]The figure showing the consistent calculation including change of the molecular dynamics simulator using the variations technique by this invention.

[Drawing 85]The figure showing the search technique by the molecular dynamics simulator by this

invention.

[Drawing 86]The characteristic figure showing the situation of the temperature setting at the time of the amorphous SiO_2 creation by this invention persons.

[Drawing 87]The characteristic figure showing the pressure variation at the time of amorphous SiO_2 creation in the computer by this invention persons.

[Drawing 88]The characteristic figure showing the volume change at the time of the amorphous SiO_2 creation by the molecular dynamics simulator which this invention persons created.

[Drawing 89]The characteristic figure showing the volume change at the time of the amorphous SiO_2 creation by the molecular dynamics simulator which this invention persons developed newly.

[Drawing 90]The characteristic figure showing the potential energy change at the time of the amorphous SiO_2 creation by the molecular dynamics simulator which this invention persons developed newly.

[Drawing 91]The characteristic figure showing the temporal change of two sides in the calculation cells at the time of the amorphous SiO_2 creation by the molecular dynamics simulator which this invention persons developed newly.

[Drawing 92]The characteristic figure showing change of the calculated energy for the molecular dynamics simulator which this invention persons developed newly using the algorithm of the usual Verlet.

[Drawing 93]The characteristic figure using the algorithm of advanced Verlet for the molecular dynamics simulator which this invention persons developed newly, and showing change of the calculated energy for it.

[Drawing 94]The characteristic figure showing the temporal change of the dipole moment calculated using the molecular dynamics simulator which this invention persons developed newly.

[Drawing 95]The characteristic figure showing the power spectrum for which this invention persons asked further from the dipole moment using the molecular dynamics simulator developed newly.

[Drawing 96]The figure applying the molecular dynamics simulator which this invention persons developed newly to alpha-SiO 2 and in which showing the calculated IR spectrum.

[Drawing 97]The figure showing the IR spectrum as which it was predicted when the molecular dynamics simulator which this invention persons developed newly was applied to alpha-SiO 2 and the external pressure was added.

[Drawing 98]The characteristic figure showing the volume change at the time of amorphous SiO by the molecular dynamics simulator which this invention persons developed newly, and creation.

[Drawing 99]The characteristic figure showing change of the calculated energy for the molecular dynamics simulator which this invention persons developed newly using the algorithm of the usual Verlet.

[Drawing 100]The figure showing the computational procedure by this invention persons.

[Drawing 101]The figure showing the computational procedure by this invention persons.

[Drawing 102]The figure showing the sliding surface in Si (100), decomposition shearing stress, etc.

[Drawing 103]The mimetic diagram showing a reaction near the SiO_2 and Si/SiO_2 interface.

[Drawing 104]The figure showing serial calculation of viscoelasticity calculation typically.

[Drawing 105]The temperature of the thickness of an oxide film, the characteristic figure showing time dependency.

[Drawing 106]The temperature of the thickness of an oxide film, the characteristic figure showing time dependency.

[Drawing 107]The temperature of the thickness of an oxide film, the characteristic figure showing time dependency.

[Drawing 108]The figure showing the principal stress distribution and maximum shear stress in trench oxidation at the time of using the doubled coefficient.

[Drawing 109]The characteristic figure showing change of the temperature which can be set like a typical heat process, and accumulation stress.

[Drawing 110]The calculation prediction figure showing distribution of sigmaxx in a trench angle.

[Drawing 111]The calculation prediction figure showing distribution of sigmaxx in a trench angle.

_____

[Translation done.]

【図132】3次元剛性マトリックスの例を示す図。

【図1】

【図4】

【図2】

【図18】　【図15】

U
-7<Qu<+1

R_A^0

原子構造モデル

【図16】

アルカリ金属
ハライド分子

【図5】

【図7】

【図12】　　【図13】　　【図14】

IP(イオン化ポテンシャル) EA(電子親和力)

【図3】

原子の座標と速度を求める

↓

電子エネルギの計算

波動方程式(KS方程式(21)、(22))を解く

基底関数：平面波(擬ポテンシャルを前提)

自己無
接着化

ポテンシャル：＿＿＿＿＿＿

電子分布の計算

電子の自己ポテンシャルの更新

↓

格子エネルギE_ωの計算

Ewald法

原子に働く力の計算

電子からの寄与：Hellman-Feynman定理

セルからの寄与：$\partial F_\omega\{R\}/\partial R$

原子の運動をふまえて
分子動力学により

原子の位置ベクトル$r(t)$、速度ベクトル$v(t)$の更新

【図9】

・ウエハーの投入

・基板前処理(クラスタツールA)

・酸化処理(クラスタツールB)

　　ガス量　　　　　Pox、△Pox

　　昇温シーケンス　Pox、△Pox

　　バルブシーケンス　Pox、△Pox

・アニールクラスタツールC

・
・
・

SiSiO₂

【図17】

電気陰性度

	Mullion	Pausing
H	7.17ev	2.1eV
B		2.0
C	5.34	2.5
N	6.90	

【図19】

C
$-4 < Q_C < +4$

【図6】

| ポテンシャルエネルギーから力を出すに当たり、計算を簡単化 | → | 2体間ポテンシャルを用いる例えば、$\propto \left(\dfrac{1}{r^6} - \dfrac{1}{r^{12}}\right)$ |

| ポテンシャルエネルギーから力を出すに当たり、計算の複雑化はそのまま | → | テーブル化して、計算の複雑さには立ち入らない |

高階巡回偏微分方程式を予め
作成計算機で高速に解を求める
(本発明)

【図10】

・ウエハーの投入

・基板前処理(クラスタツールA)

・強誘電性スパッタ(クラスタツールB)

　　電源電圧

　　ターゲット電圧

　　スパッタ時間

　　バルブシーケンス

・アニールクラスタツールC

・
・
・

未使用材料

【図８】

【図１１】

【図２０】

O
-2<Q₀<+6

【図２１】

【図２２】

【図23】

```
        ┌─────────┐
        │  START  │
        └────┬────┘
   ┌─────────────────────┐
   │ SiO2等寄構造データ入力  │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │    計算条件の入力     │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │   各原子の特性を設定   │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │ 電荷、水素補正電荷の初期化 │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │ 係数マトリックスC、      │
   │ ベクトルdの設定         │
   └─────────┬───────────┘
   ┌─────────────────────┐         ┌──────────────┐
   │  マトリックスのLU分解   │         │ エワルド項を再計算し │
   └─────────┬───────────┘         │ マトリックスを変更  │
   ┌─────────────────────┐         └──────────────┘
   │   マトリックスを解く    │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │   水素電荷の収束判断    │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │   境界条件のチェック    │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │    ピボットの選択      │
   └─────────┬───────────┘
   ┌─────────────────────┐
   │    計算結果の出力      │
   └─────────┬───────────┘
        ┌────┴────┐
        │   END   │
        └─────────┘
```

【図25】

```
   ┌─────────────────────┐
   │      酸化・拡散        │
   ├─────────────────────┤
   │      分散・変動        │
   └─────────────────────┘
   ┌─────────────────────┐
   │      イオン注入        │
   ├─────────────────────┤
   │      分散・変動        │
   └─────────────────────┘
   ┌─────────────────────┐
   │      リソグラフィ       │
   ├─────────────────────┤
   │      分散・変動        │
   └─────────────────────┘
   ┌─────────────────────┐
   │     CVD・エッチング     │
   ├─────────────────────┤
   │      分散・変動        │
   └─────────────────────┘
   ┌─────────────────────┐
   │      気相成長         │
   ├─────────────────────┤
   │      分散・変動        │
   └─────────────────────┘
   ┌─────────────────────┐
   │      未知材料         │
   ├─────────────────────┤
   │      諸特性算出        │
   └─────────────────────┘
```

【図26】

酸化時間経過	正常プロセス 1000℃	変動プロセス 1005℃
t_1	D_1 ϕ_1 C_1 →	ΔC_1
t_2	Nowton法	
	$F(C) = B \cdot A^{k+1}$ $\Delta C^{k+1} = -\dfrac{1}{\Delta t} \Delta C^k - \Delta A \cdot C^{k+1}$	
t_{n-1}	D^{n-1} ϕ^{n-1} C^{n-1} →	ΔC^{n-1}
t_n	D^n ϕ^n C^n →	ΔC^n

【図27】

縦軸: 残差、横軸: 反復回数

(100) ボロン
ボロン イオン注入
40kv, 6×10^{12}/cm^2
ロコス 1000℃, 1H
正常プロセス
1回目ニュートンループ
2回目ニュートンループ
3回目ニュートンループ
新しいニュートンループ
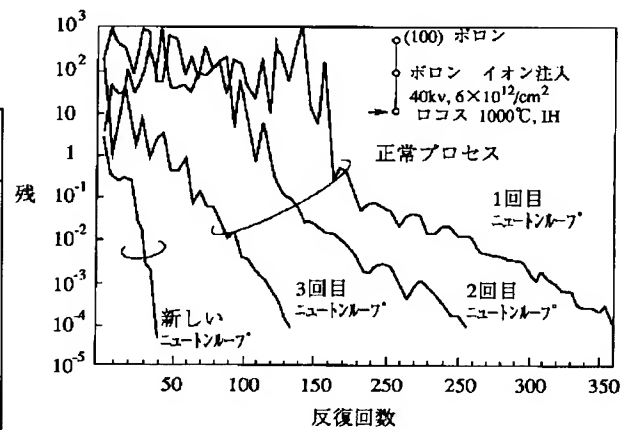
【図24】

Tnでの結合角

BOND ANGLES AT SI ATOM		AT TIME	(FS)						
0 -	SI -	0	(DEGREE)	0 -	SI -	0	(DEGREE)	0 -	SI -	0	(DEGREE)
1-	1-	2	108.9349	1-	1-	28	108.5615	1-	1-	103	109.4750
2-	1-	28	110.2779	2-	1-	103	109.5298	28-	1-	103	110.0363
1-	2-	3	108.9505	1-	2-	4	110.6575	1-	2-	70	110.2105
3-	2-	4	108.8379	3-	2-	70	109.2018	4-	2-	70	108.9536
3-	3-	5	109.9244	3-	3-	6	109.6437	3-	3-	16	109.9806
5-	3-	6	110.0583	5-	3-	16	108.3414	6-	3-	16	108.8641
5-	4-	7	109.3194	5-	4-	8	110.0928	5-	4-	130	109.9225
7-	4-	8	109.7291	7-	4-	130	109.2644	8-	4-	130	108.4557
4-	5-	9	109.3677	4-	5-	10	110.5243	4-	5-	111	109.8644
9-	5-	10	110.9178	9-	5-	111	108.1002	10-	5-	111	108.0205
9-	6-	11	110.1572								
11-	6-	12	110.2308								
11-	7-	13	111.1628								
13-	7-	14	108.8920								
13-	8-	15	109.3806								
15-	8-	16	109.6320								
12-	9-	17	108.3242								
17-	9-	18	108.6424								
17-	10-	19	107.7255								
19-	10-	20	110.5358								
19-	11-	21	108.8805								
21-	11-	22	110.1516								
21-	12-	23	110.0312								
23-	12-	24	109.5848								
20-	13-	25	110.5169								
25-	13-	26	110.3303								
25-	14-	27	109.1309								
27-	14-	28	109.2992								
8-	15-	27	110.1251								
27-	15-	29	110.7322								
29-	16-	31	109.6533								
31-	16-	32	108.5453								
33-	17-	34	109.8139								
34-	17-	60	110.1016								
6-	18-	33	109.3102								
33-	18-	35	110.2591								
35-	19-	37	108.9678								
37-	19-	38	109.7983								
37-	20-	39	109.8264								
39-	20-	40	108.8545								
36-	21-	41	109.0508								
41-	21-	42	109.9605								
14-	22-	41	110.3527								
41-	22-	43	109.3678								
43-	23-	45	110.8370								
45-	23-	46	107.8368								
45-	24-	47	110.7456								
47-	24-	48	108.6719								
44-	25-	49	110.6992								
49-	25-	50	109.1146								
22-	26-	49	110.3576								
49-	26-	51	110.6860								
51-	27-	53	111.4685								
53-	27-	54	109.8225								
53-	28-	55	109.2661								
55-	28-	55	109.5974								

Tnでの結合長

BOND ANGLES AT SI ATOM		AT TIME	(FS)		
0 -	SI	(ANGSTROM)	0 -	SI	(ANGSTROM)	0 -	SI
1 -	1	1.6503	1 -	2	1.5914		
2 -	1	1.6132	2 -	84	1.6149		
3 -	2	1.5863	3 -	3	1.6158		
4 -	2	1.6175	4 -	5	1.5837		
5 -	3	1.6088	5 -	4	1.6121		
6 -	3	1.6093	6 -	18	1.6181		
7 -	4	1.6241	7 -	49	1.5875		
8 -	4	1.6303	8 -	15	1.6090		
9 -	5	1.5924	9 -	1	1.5555		
10 -	5	1.5842					
11 -	6	1.5857					
12 -	6	1.6054					
13 -	7	1.6014					
14 -	7	1.6182					
15 -	8	1.5887					
16 -	3	1.6306					
17 -	9	1.6182					
18 -	9	1.6174					
19 -	10	1.6056					
20 -	10	1.6132					
21 -	11	1.5974					
22 -	11	1.6070					
23 -	12	1.5951					
24 -	7	1.6219					
25 -	13	1.5883					
26 -	13	1.6273					
27 -	14	1.6136					
28 -	1	1.5151					
29 -	15	1.6091					
30 -	15	1.6199					
31 -	16	1.6161					
32 -	11	1.5255					
33 -	17	1.6316					
34 -	17	1.5912					
35 -	18	1.6193					
36 -	18	1.5952					
37 -	19	1.5452					
38 -	19	1.5997					
39 -	20	1.6350					
40 -	20	1.6094					
41 -	21	1.5020					

Tn+1での結合角

BOND ANGLES AT SI ATOM					SI -
SI -	0 -	SI	(DEGREE)		
1-	1-	2	141.9792		
1-	2-	84	141.6846		
2-	3-	3	143.3545		
2-	4-	5	144.2273		
3-	5-	4	141.0583		
3-	6-	18	143.0912		
4-	7-	49	142.8356		
4-	8-	15	142.2639		
5-	9-	6	144.0091		
5-	10-	83	141.1559		
6-	11-	7	143.1985		
6-	12-	9	143.4654		
7-	13-	8	142.7547		
7-	14-	22	143.7993		
8-	15-	53	143.7927		
3-	16-	8	142.6664		
9-	17-	10	142.0174		
9-	18-	92	143.2893		
10-	19-	11	143.0853		
10-	20-	13	140.8887		
11-	21-	12	142.2522		
11-	22-	26	143.9689		
12-	23-	57	142.1776		
7-	24-	12	142.7455		
13-	25-	14	142.4813		
13-	26-	96	141.4551		
14-	27-	15	143.1551		
1-	28-	14	142.8827		

Tn+1での結合長

BOND LEN	
0 -	SI
1-	1
2-	1
3-	2
4-	2
5-	3
6-	3
7-	4
8-	4
9-	5
10-	5
11-	6
12-	6
13-	7
14-	7
15-	8
16-	8
17-	9
18-	9
19-	10
20-	10
21-	11
22-	11
23-	12
24-	7

【図117】

素子領域　素子分離絶縁膜　Si基板

【図118】

ゲート熱酸化膜　素子分離絶縁膜　Si基板

【図２８】

```
*** CONCENT     BORON ***
        I=  1         2         3         4         5         6         7         8         9
K=  1 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1
    2 5.704E+14 5.704E+14 6.270E+14 6.596E+14 7.484E+14 8.005E+14 8.402E+14 8.549E+14 9.094E+14 9
    3 5.704E+14 5.704E+14 6.270E+14 6.596E+14 7.484E+14 8.005E+14 9.105E+14 9.549E+14 9.094E+14
    4 6.063E+14 6.063E+14 6.596E+14 7.390E+14 8.043E+14 8.632E+14 9.093E+14 9.334E+14 9.093E+14
    5 6.344E+14 6.344E+14 7.621E+14 8.470E+14 9.274E+14 9.995E+14 1.060E+15 1.101E+15 1.112E+15
    6 9.174E+14 9.174E+14 9.193E+14 1.011E+15 1.136E+15 1.231E+15 1.313E+15 1.379E+15 1.425E+15
    7 1.022E+15 1.035E+15 1.169E+15 1.322E+15 1.447E+15 1.594E+15 1.713E+15 1.814E+15 1.896E+15
    8 1.353E+15 1.353E+15 1.557E+15 1.774E+15 1.953E+15 2.171E+15 2.332E+15 2.465E+15 2.613E+15
    9 1.875E+15 1.874E+15 2.170E+15 2.470E+15 2.792E+15 3.067E+15 3.316E+15 3.535E+15 3.728E+15
   10 2.697E+15 2.697E+15 3.143E+15 3.625E+15 4.052E+15 4.492E+15 4.872E+15 5.204E+15 5.497E
   11 4.030E+15 4.030E+15 4.722E+15 5.467E+15 6.173E+15 6.517E+15 7.393E+15 7.909E+15 8.361E
   12 6.231E+15 6.231E+15 7.323E+15 8.509E+15 9.625E+15 1.065E+16 1.154E+16 1.237E+16 1.309E
   13 9.922E+15 9.922E+15 1.170E+16 1.361E+16 1.542E+16 1.707E+16 1.855E+16 1.986E+16 2.102
   14 1.619E+16 1.619E+16 1.913E+16 2.225E+16 2.524E+16 2.795E+16 3.042E+16 3.252E+16 3.44
   15 2.690E+16 2.690E+16 3.183E+16 3.710E+16 4.208E+16 4.663E+16 5.071E+16 5.433E+16 5.75
   16 4.513E+16 4.513E+16 5.331E+16 6.241E+16 7.032E+16 7.367E+16 8.537E+16 9.147E+16 9.67
   17 7.602E+16 7.602E+16 9.010E+16 1.051E+17 1.193E+17 1.322E+17 1.435E+17 1.541E+17 1.6
   18 1.266E+17 1.266E+17 1.502E+17 1.751E+17 1.952E+17 2.205E+17 2.399E+17 2.571E+17 2.7
   19 2.055E+17 2.055E+17 2.442E+17 2.830E+17 3.235E+17 3.548E+17 3.901E+17 4.180E+17 4.
   20 3.201E+17 3.201E+17 3.793E+17 4.436E+17 5.033E+17 5.577E+17 6.069E+17 6.503E+17 6.
   21 4.647E+17 4.647E+17 5.519E+17 6.443E+17 7.312E+17 8.105E+17 8.817E+17 9.445E+17 1.
   22 6.113E+17 6.113E+17 7.260E+17 8.474E+17 9.615E+17 1.066E+18 1.160E+18 1.243E+18 1
   23 7.004E+17 7.004E+17 8.311E+17 9.707E+17 1.102E+18 1.221E+18 1.328E+18 1.423E+18 1
   24 6.651E+17 6.651E+17 7.895E+17 9.217E+17 1.046E+18 1.160E+18 1.261E+18 1.352E+18 1
   25 4.921E+17 4.921E+17 5.842E+17 6.820E+17 7.741E+17 8.551E+17 9.314E+17 1.000E+18 1.
   26 2.539E+17 2.539E+17 3.073E+17 3.585E+17 4.072E+17 4.514E+17 4.910E+17 5.262E+17 5.
   27 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.
```

【図２９】

```
*** CONCENT     BORON ***
        I=  1         2         3         4         5         6         7         8         9
K=  1 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.000E+14 1.
    2 5.745E+14 5.745E+14 6.315E+14 6.945E+14 7.542E+14 8.047E+14 8.473E+14 8.605E+14 8.051E+14 9.
    3 5.745E+14 5.745E+14 6.315E+14 6.745E+14 7.542E+14 8.069E+14 8.473E+14 9.090E+14 9.051E+14 9
    4 6.105E+14 6.105E+14 6.742E+14 7.443E+14 8.107E+14 8.697E+14 9.165E+14 9.397E+14 9.145E+14 9
    5 6.223E+14 6.223E+14 7.670E+14 8.526E+14 9.337E+14 1.005E+15 1.067E+15 1.107E+15 1.113E+15 1
    6 9.223E+14 9.223E+14 9.251E+14 1.037E+15 1.143E+15 1.239E+15 1.322E+15 1.375E+15 1.432E+15
    7 1.035E+15 1.035E+15 1.175E+15 1.330E+15 1.463E+15 1.605E+15 1.725E+15 1.824E+15 1.906E+15
    8 1.366E+15 1.366E+15 1.567E+15 1.783E+15 1.994E+15 2.183E+15 2.352E+15 2.495E+15 2.627E+15
    9 1.933E+15 1.933E+15 2.131E+15 2.302E+15 2.607E+15 3.043E+15 3.334E+15 3.536E+15 3.747E+1
   10 2.711E+15 2.711E+15 3.159E+15 3.453E+15 4.101E+15 4.520E+15 4.890E+15 5.230E+15 5.523E+1
   11 4.051E+15 4.051E+15 4.744E+15 5.492E+15 6.200E+15 6.847E+15 7.428E+15 7.944E+15 8.399E
   12 6.261E+15 6.261E+15 7.359E+15 8.544E+15 9.666E+15 1.069E+16 1.161E+16 1.242E+16 1.314E
   13 9.965E+15 9.965E+15 1.174E+16 1.366E+16 1.547E+16 1.713E+16 1.861E+16 1.943E+16 2.130E
   14 1.625E+16 1.625E+16 1.919E+16 2.235E+16 2.534E+16 2.804E+16 3.051E+16 3.265E+16 3.460E
   15 2.699E+16 2.699E+16 3.191E+16 3.739E+16 4.219E+16 4.673E+16 5.083E+16 5.447E+16 5.767
   16 4.531E+16 4.531E+16 5.363E+16 6.254E+16 7.044E+16 7.866E+16 8.554E+16 9.166E+16 9.70
   17 7.817E+16 7.817E+16 9.026E+16 1.053E+17 1.195E+17 1.324E+17 1.441E+17 1.544E+17 1.63
   18 1.269E+17 1.269E+17 1.504E+17 1.755E+17 1.971E+17 2.207E+17 2.401E+17 2.573E+17 2.7
   19 2.061E+17 2.061E+17 2.446E+17 2.852E+17 3.237E+17 3.525E+17 3.905E+17 4.183E+17 4.4
   20 3.204E+17 3.204E+17 3.800E+17 4.435E+17 5.034E+17 5.525E+17 6.070E+17 6.505E+17 6.
   21 4.652E+17 4.652E+17 5.519E+17 6.443E+17 7.312E+17 8.105E+17 8.816E+17 9.445E+17 1.
   22 6.117E+17 6.117E+17 7.259E+17 8.472E+17 9.616E+17 1.066E+18 1.159E+18 1.243E+18 1
   23 7.006E+17 7.006E+17 8.311E+17 9.704E+17 1.101E+18 1.221E+18 1.323E+18 1.423E+18 1
   24 6.653E+17 6.653E+17 7.895E+17 9.215E+17 1.046E+18 1.159E+18 1.261E+18 1.351E+18 1
   25 4.924E+17 4.924E+17 5.843E+17 6.820E+17 7.740E+17 8.520E+17 9.333E+17 1.000E+18 1
   26 2.571E+17 2.571E+17 3.074E+17 3.585E+17 4.072E+17 4.514E+17 4.910E+17 5.262E+17 5.
   27 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.500E+14 2.
```

【図３０】

```
** SODP K    BORON ***              DELTA T = 1.000E+00
     I=   1         2         3         4         5         6         7         8         9
 X= 1 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.
    2 3.935E+12 3.935E+12 4.353E+12 4.965E+12 5.570E+12 6.056E+12 6.231E+12 7.035E+12 5.111E+12 6.
    3 3.935E+12 3.935E+12 4.352E+12 4.965E+12 5.570E+12 6.056E+12 6.281E+12 7.035E+12 5.111E+12 6.
    4 4.002E+12 4.002E+12 4.407E+12 5.022E+12 5.635E+12 6.132E+12 6.384E+12 7.206E+12 5.450E+12 6.
    5 4.271E+12 4.271E+12 4.674E+12 5.312E+12 5.967E+12 6.510E+12 6.833E+12 6.305E+12 6.346E+12 .
    6 4.871E+12 4.871E+12 5.294E+12 6.012E+12 6.749E+12 7.389E+12 7.639E+12 8.017E+12 7.907E+12 .
    7 5.937E+12 5.937E+12 6.410E+12 7.268E+12 8.146E+12 8.969E+12 9.610E+12 1.006E+13 1.023E+13 .
    8 7.644E+12 7.644E+12 3.203E+12 9.266E+12 1.044E+13 1.149E+13 1.260E+13 1.313E+13 1.370E+13 .
    9 1.024E+13 1.024E+13 1.092E+13 1.235E+13 1.388E+13 1.531E+13 1.658E+13 1.747E+13 1.861E+13 .
   10 1.411E+13 1.411E+13 1.493E+13 1.687E+13 1.893E+13 2.092E+13 2.289E+13 2.424E+13 2.584E+13 .
   11 1.984E+13 1.984E+13 2.065E+13 2.347E+13 2.633E+13 2.909E+13 3.157E+13 3.374E+13 3.574E+13 .
   12 2.327E+13 2.327E+13 2.962E+13 3.303E+13 3.704E+13 4.087E+13 4.435E+13 4.747E+13 5.024E+13 .
   13 4.066E+13 4.066E+13 4.175E+13 4.667E+13 5.229E+13 5.767E+13 6.257E+13 6.695E+13 7.081E+13 .
   14 5.857E+13 5.857E+13 5.914E+13 6.575E+13 7.352E+13 8.105E+13 8.792E+13 9.403E+13 9.948E+13
   15 8.396E+13 8.396E+13 8.245E+13 9.145E+13 1.021E+14 1.124E+14 1.217E+14 1.302E+14 1.377E+14
   16 1.185E+14 1.185E+14 1.152E+14 1.236E+14 1.374E+14 1.510E+14 1.635E+14 1.747E+14 1.84E+14
   17 1.623E+14 1.623E+14 1.673E+14 1.587E+14 1.754E+14 1.923E+14 2.075E+14 2.212E+14 2.3E+14
   18 2.120E+14 2.120E+14 1.787E+14 1.365E+14 2.040E+14 2.225E+14 2.395E+14 2.553E+14 2.7E+14
   19 2.573E+14 2.573E+14 1.905E+14 1.166E+14 2.156E+14 2.307E+14 2.446E+14 2.
   20 2.813E+14 2.113E+14 1.541E+14 1.315E+14 1.309E+14 1.359E+14 1.414E+14 1.470E+14 1.
   21 2.693E+14 2.693E+14 5.973E+13 4.077E+12-2.260E+13-3.905E+13-5.211E+13-6.343E+13-7.
   22 2.261E+14 2.261E+14-5.723E+13-1.680E+14-2.270E+14-2.708E+14-3.082E+14-3.411E+14
   23 1.911E+14 1.911E+14-1.430E+14-2.837E+14-3.441E+14-4.261E+14-4.797E+14-5.271E+14
   24 2.123E+14 2.123E+14-1.012E+14-2.281E+14-2.987E+14-3.523E+14-3.984E+14-4.391E+14
   25 2.595E+14 2.595E+14 4.421E+13-3.003E+13-6.297E+13-8.479E+13-1.026E+14-1.182E+14
   26 1.490E+14 1.490E+14 6.087E+13 2.843E+13-1.742E+13 1.221E+13-4.383E+12 5.200E+12 .
   27 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.
```

【図３１】
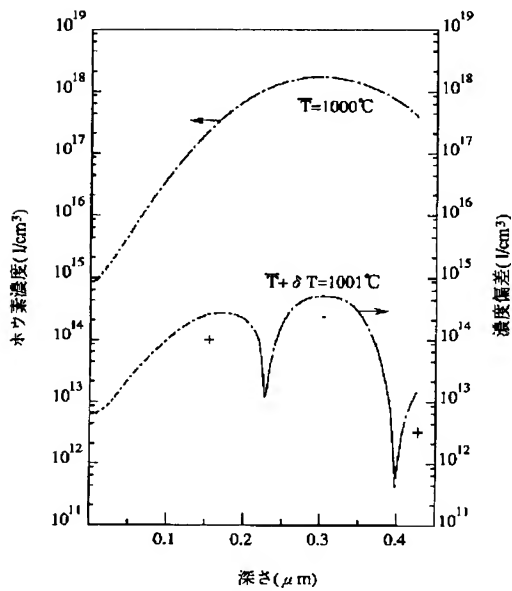
【図３２】

```
U α  (0.025)      CU   α β  (0.02375)      UCC  α β γ  (0.0226)
C α  (0.95)       UC   α β  (0.02375)      CCU  α β γ  (0.0226)
L α  (0.025)      CC   α β  (0.9025)       CUC  α β γ  (0.0226)
                  LC   α β  (0.02375)      CCC  α β γ  (0.8574)
                  CL   α β  (0.02375)      CCL  α β γ  ( ・ )
                                           CLC  α β γ  ( ・ )
                                           LCC  α β γ  ( ・ )
```

```
⎧ U  Upper   度数   0.025
⎨ C  Center  度数   0.95
⎩ L  Lower   度数   0.025
```

【図３８】

(a) BaTiO₃　　　　(b) PbTiO₃

【図５０】

【図33】

検定始め

予と実の最大値を比較

|実−予| ≤ ε ?

YES → "異常はないよう" → 別の枝に進む

NO → "酸化/拡散工程に異常がありそう"

予:実

> "酸化時間が長いか、温度が高かったようだ" → 予と実の位置を比較

< "酸化時間が短かいか、温度が低かったようだ" → 予と実の位置を比較

|実−予| < ε ?
YES → 接合は適切
NO → 実:予
> 接合位置が予測より深いようだ温度が高い → LOADモジュールを実行
< 浅いようだ酸化工程が長い → LOADモジュールを実行

|実−予| < ε ?
YES → 接合位置はOK
NO → 実:予
> 接合位置が深いようだ温度が低い → LOADモジュールを実行
< 浅いようだ工程が短かい → LOADモジュールを実行

【図34】

O Ti Sr
Ti O Sr
Si
c軸
a軸
Ti
O

【図42】

Ti
O
Pb

【図35】

新分子動力学シミュレータ

イオン・共存結合型分子動力学

②

共有結合型分子動力学

①

DFT
EIGEN

CRYST
SiO₂結晶ルーチン

UNIT
単位ルーチン

TETRA
4面体構造ルーチン

EWALD
Ewaldプログラム

RHOMBO
ロンボ構造

DIAMOND
ダイヤモンド構造

TERSOFF
Si分子間ポテンシャル計算

PREPAR
前処理ルーチン

NEIBOR
極近場分子の番号付

HSORT

MAXWELL
マクスウェル分布

【図44】

Ti
O
Pb

【図３６】

【図３７】

ベロブスカイトPbTiO₃結晶構造

【図３９】

【図４０】

【図４３】

【図４１】

【図４５】

欠損
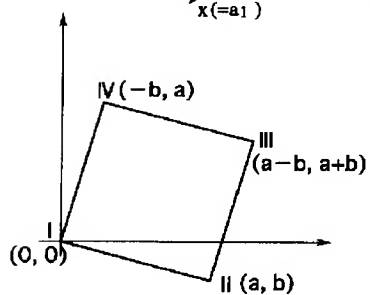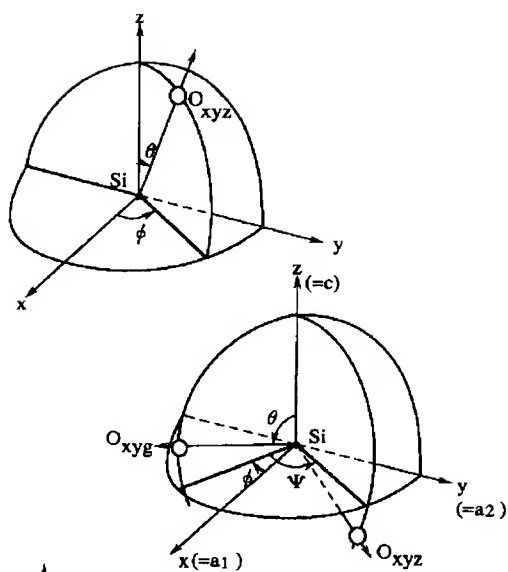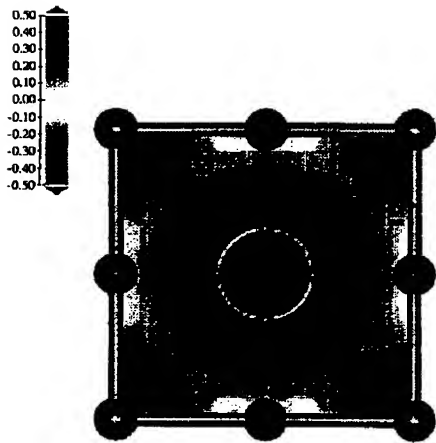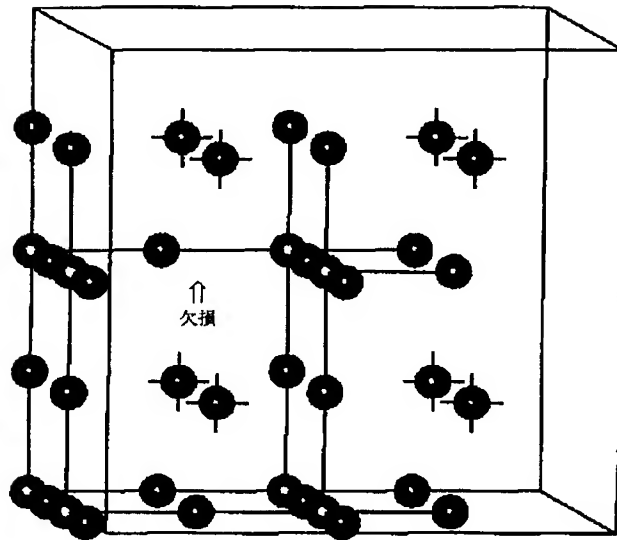
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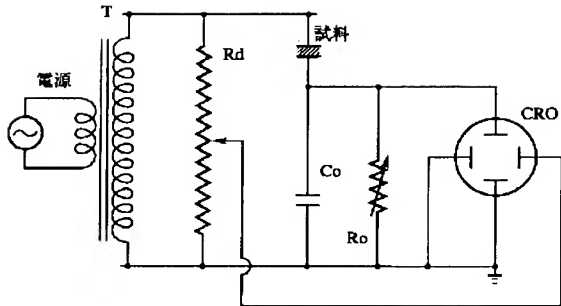
【図４８】
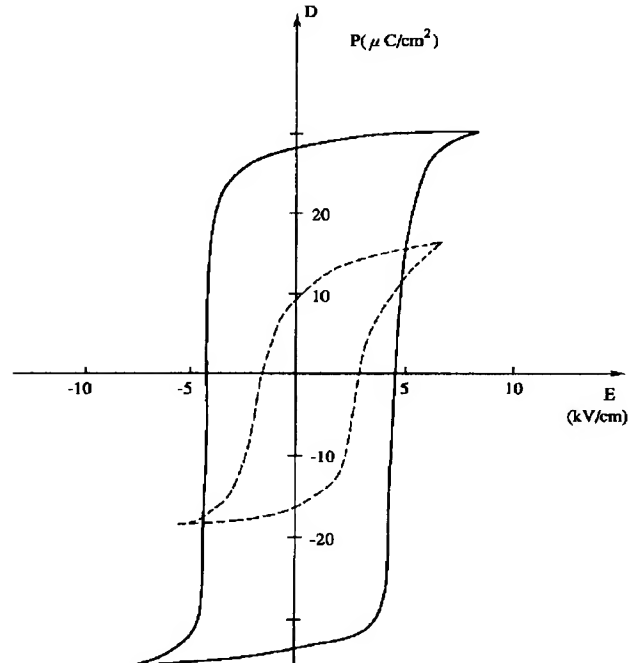
【図５３】
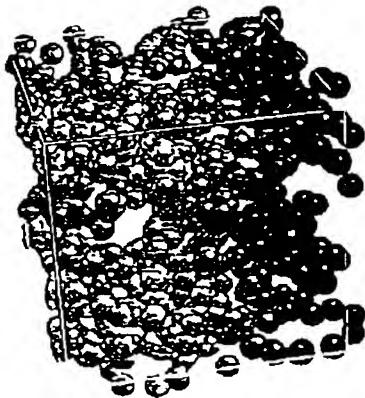
【図４６】

tmp-PbTiO₃

```
Cartesian coordinates (bohr)
7.36991773809233E+00    3.68503830556782E+00    7.36999010703879E+00
3.68492904917006E+00    7.36990675500488E+00    7.36998965539427E+00
1.85344324959821E-05    1.45452209340920E-05    3.40147019434692E+00
6.37215603348813E-05    7.36992081267651E+00    3.51659109214652E-05
3.68493242800013E+00    3.68491260288479E+00    3.96842529600134E+00
Cartesian forces (hart/bohr); max,rms= 1.43767E-02 4.51782E-03 (unfixed atoms)
-1.80940035404206E-04   -2.07537373211315E-04   -2.04964454194065E-03
 2.56880079450442E-04    4.07888591617262E-05   -2.14973113771572E-03
 2.24243540544528E-05    1.10425697382921E-04   -6.93585136915477E-04
-2.24118747243653E-04   -2.11855686110157E-05   -9.48369575837913E-03
 1.25754349142964E-04    7.75083852776827E-05    1.43766565749510E-02

Cartesian coordinates (bohr)
7.36973679805692E+00    3.68483076819461E+00    7.36794046249685E+00
3.68518592924951E+00    7.36994754386404E+00    7.36783992425656E+00
4.09587865504349E-05    1.24970918317013E-04    3.40077660921001E+00
-1.60397186908771E-04    7.36989962710790E+00   -9.44852984745766E-03
3.68505818234927E+00    3.68499011127006E+00    3.98280195257629E+00
Cartesian forces (hart/bohr); max,rms= 8.34605E-03 2.45956E-03 (unfixed atoms)
-1.61895617366627E-05    3.09255883087009E-06   -1.19915787731153E-03
 7.34168075079671E-05    1.12756648306686E-04   -1.10022284067273E-03
-2.24275552232517E-05   -2.41956035453473E-05   -3.24637418523411E-03
 1.06415727261410E-04   -2.44007083322998E-05   -2.80029696512406E-03
-1.41215417809463E-04   -6.72528952599095E-05    8.34605186834244E-03

Cartesian coordinates (bohr)
7.36967174041861E+00    3.68479961773717E+00    7.36516510152224E+00
3.68537949760620E+00    7.37018116183304E+00    7.36524508710990E+00
-1.16727938556601E-08    9.62925456730003E-05    3.39413705673712E+00
1.28129761298314E-05    7.36984684725815E+00   -1.67751205094258E-02
3.68479743192721E+00    3.68486910198090E+00    4.00213829383241E+00
Cartesian forces (hart/bohr); max,rms= 7.20602E-03 2.08967E-03 (unfixed atoms)
 1.28850801532736E-04    7.06412663085704E-05   -1.50295459585843E-03
-1.58012861369054E-04   -1.74164668147622E-04   -1.46956505541997E-03
 7.08589715586290E-05    5.67021085975686E-06   -2.28610955944484E-03
-1.73598433456127E-04    8.43701157472647E-05   -1.94739350275452E-03
 1.31901896135616E-04    1.34830752320297E-05    7.20602271347777E-03


Cartesian coordinates (bohr)
7.37021318634145E+00    3.68505926267177E+00    7.34658602343312E+00
3.68506431084086E+00    7.36978023696826E+00    7.34735839048843E+00
3.39286295583846E-04    9.97498200251742E-05    3.35993819043655E+00
-6.84291357691068E-04    7.37021688700809E+00   -5.49264155838585E-02
3.68492897913516E+00    3.68463688488677E+00    4.11095422991800E+00
Cartesian forces (hart/bohr); max,rms= 1.40552E-02 5.32522E-03 (unfixed atoms)
-1.54149077482324E-04   -1.38672668831043E-04    2.44677120516630E-03
 4.19884602629664E-04    1.54548773067693E-04    2.36496445003840E-03
-2.41608460357061E-05   -2.57753838330758E-05   -5.07590096094921E-03
-1.73065113649408E-04   -3.18303354074471E-05    1.40552397966281E-02
-6.85095654622252E-05    4.17296150038733E-05   -1.37910744908836E-02

bravais matrix for conventional unit cell in Angstroms is:

      a1         a2         a3
   3.90000    0.00000    0.00000
   0.00000    3.90000    0.00000
   0.00000    0.00000    4.20000


rms force= 5.3252E-03 > tolerance ftoler= 2.0000E-03 hart/bohr (unfixed atoms)
```

【図49】

In-situ 測定装置

入力ガス構成分析
反応ガス組成分析

XPS
FT-IR
TEM

時間・空間内での
運動量 ---- 等の分散

【図51】

【図52】

【図54】

Si 32個
O 64個
逆格子 520点
温度 1000K
Δt 0.2ff

Si-o-Si 角度(度)

#6
#9
#15
#40
#3

120

50100 50200 50300 50400

時間(fs)

【図71】

ラマンスペクトル(VV分極)

VV

a

b

0 200 400 600 800 1000 1200

ラマンシフト(cm⁻¹)

【図55】

温度の時間依存性

Si(100)バルク <npt>.M=1e11kg/m4

T(K)

Pc = -7.5e9Pa

4000

3000

2000

1000

0

温度

0 2000 4000 6000 8000 10000 12000

時間(fs)

【図56】

γ c=2.75Å, c - Si, T=1687K.

n
150

100

50

0

0 20 40 60 80 100 120 140 160 180

結合角(度)
結合角分布

【図73】

強度(a.u.)

―― 0%応力
---- 3.5%応力

300 600 900

ラマンシフト(cm⁻¹)

【図５７】

g(r)　　　　c-Si　T=1687K　no.1.

Si－Si間距離 r(Å)
g(r)

【図５８】

g(r)　　　　melt Si　T=1850K.

r(A)
g(r)関数

【図５９】

g(r)　　　　I－Si　T=1687K.

r(A)
g(r)関数

【図６０】

n
γ c＝2.75Å melt Si, T=2687K.

結合角(度)
結合角分布

【図７４】

(a)　　　　　　　(b)

ストレスなし　　　ストレスあり

$\psi 0$　　　　　　　α

－軸ストレス

β

ψ＝109.5°　　　$\alpha > \psi > \beta$

【図61】

g(r)　　　　　　　　I - Si T=2687K.

g(r)関数

【図62】

g(r)　　　　　　　　a - Si T=1187K.

g(r)関数

【図63】

n　　　　　　a - Si SPE, T=6000C, 時間=70psec

結合角(度)
結合角分布

【図64】

n　　　　　　a - Si SPE, T=600C, 時間=80psec.

結合角(度)
結合角分布

【図81】

オキシナイトライドによってX線の強度が減少

SiO₂

オキシナイトライド

オキシナイトライド

SiO2

Si-Si結合　　　Si-O結合

X線の強度(単位は任意)

X線のエネルギー(keV)

【図104】

応力
σ

(1)　(2)　(3)　(4)

0　　0.002分後　0.003分後

所定酸化工程時間

【図６５】

a‐Si SPE, T=600C, 時間=90psec.

結合角(度)
結合角分布

【図６６】

SPE T=600C, 70psec.

r(A)
g(r)関数

【図６７】

SPE T=600C, 80psec.

r(A)
g(r)関数

【図６８】

SPE T=600C, 90psec.

r(A)
g(r)関数

【図６９】

a - Si T=472K no.2.

g(r)関数

【図７２】

【図７０】

【図75】

(a)

【図76】

(b)

ストレスなし振動

(c)

ストレス

【図80】

(a)   (b)

【図77】

298K 30000 0.05fs latm. out 1

【図78】

【図85】

【図79】

【図82】

NORPROM 16min

(a)

距離(μm)

距離(μm)

1.8e+0.9
1.08e+0.9
-3.6e+0.8
-1.08e+0.9
-1.8e+0.9

NORPROM 40Mmin

(b)

1.8e+0.9
1.08e+0.9
-3.6e+0.8
-1.08e+0.9
-1.8e+0.9

距離(μm)

【図83】

本発明
電荷未改良

本発明
電荷改良

k(cm⁻¹)

【図91】

y(A)

SiO₂

x(A)

【図84】

| ···· | -δp | -δta | C工程 | +δta | +δp | ···· |

····

| | | D工程 | | | ···· |

【図86】

T(K)

6000

SiO₂

温度

4000

2000

0

0　　200　　400　　600　　800　　1000

時間(fs)

【図102】

分解剪断応力

(111)面

(110)面

【図103】

C

D'(σ)

k's(σ)

U

μ

k's(h,k,l)

Si

SiO₂

【図87】

1.5

SiO₂

P(×10⁻¹⁰Pa)

圧力

1.0

0.5

0

0　　200　　400　　600　　800　　1000

時間(fs)

【図８８】

V(×1000 A3)　　　　　　　　　SiO₂

【図９９】

【図８９】

V(×1000 Å3)　　　　　　　SiO₂

【図９０】

【図１０８】

(a)

(b)

最大剪断応力

【図９２】

【図９３】

【図１１９】

【図９４】

【図９８】

【図９５】

【図９６】
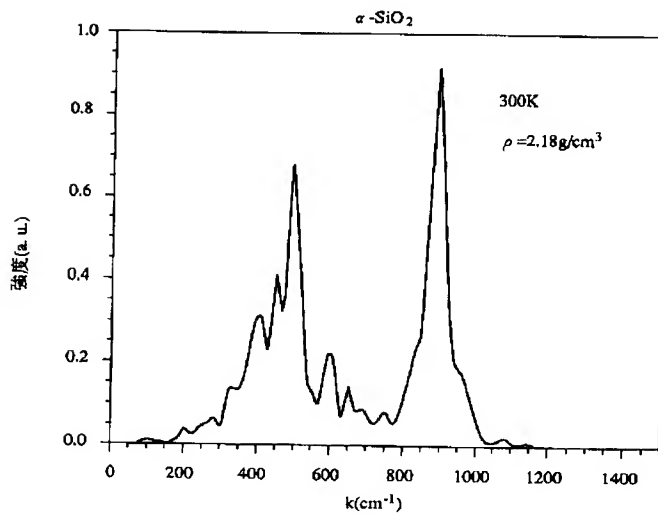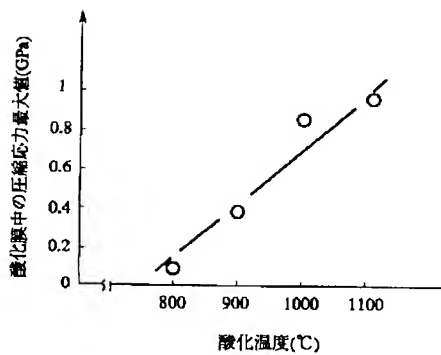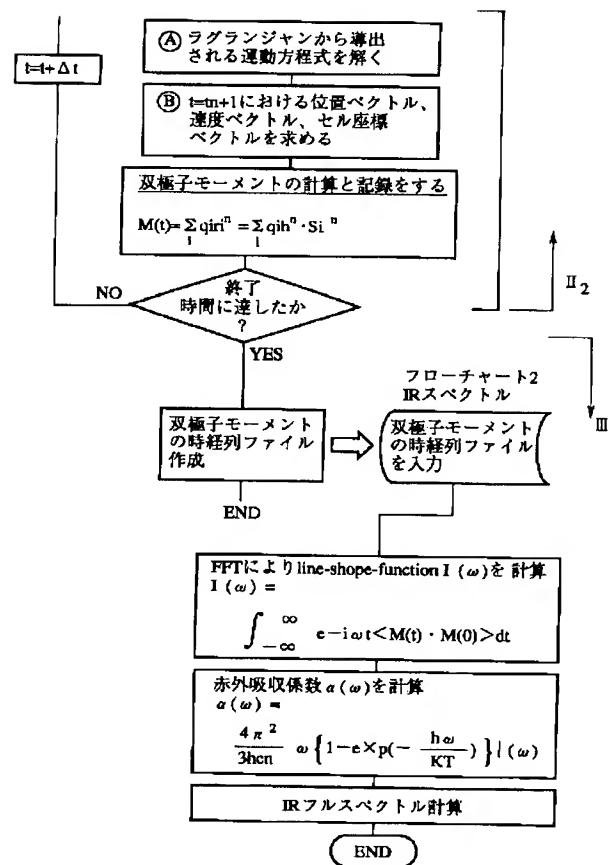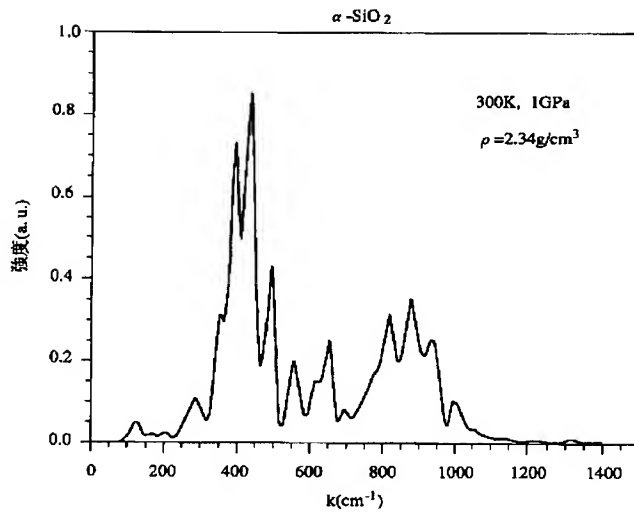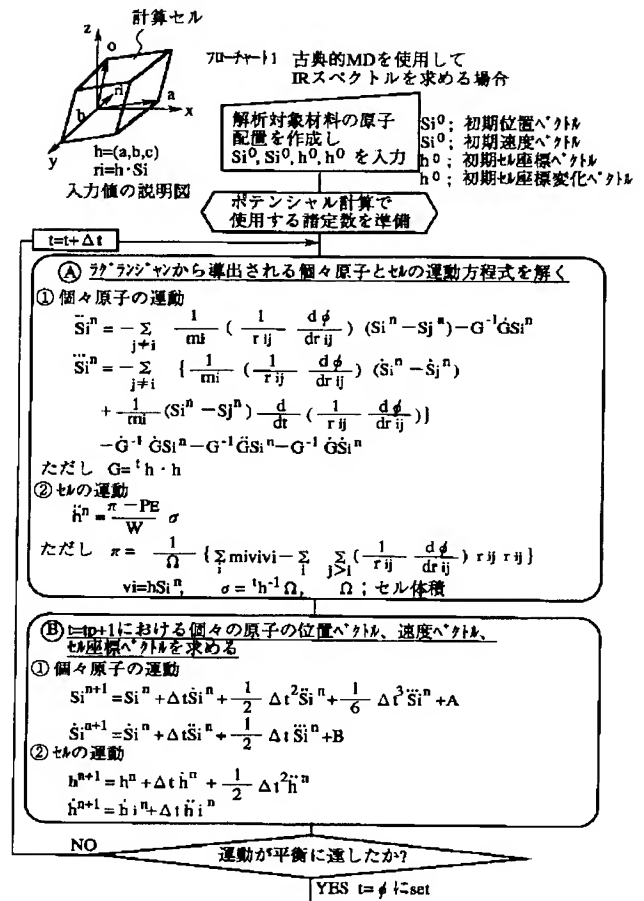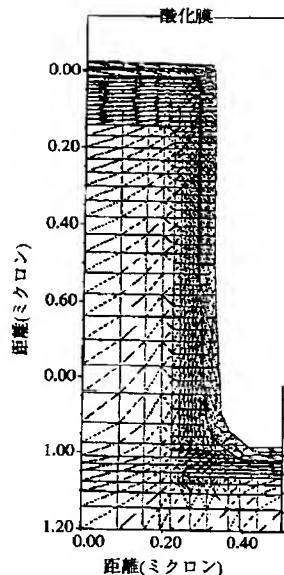
α -SiO$_2$

300K

ρ =2.18g/cm^3

【図１２３】

【図１０１】

Ⓐ ラグランジャンから導出される運動方程式を解く

Ⓑ t=tn+1における位置ベクトル、速度ベクトル、セル座標ベクトルを求める

双極子モーメントの計算と記録をする

$M(t)= \sum_i q_i r_i^n = \sum_i q_i h^n \cdot S_i^n$

終了時間に達したか？

NO

YES

双極子モーメントの時経列ファイル作成

END

フローチャート２
IRスペクトル

双極子モーメントの時経列ファイルを入力

FFTにより line-shope-function I (ω) を計算

$I(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} <M(t) \cdot M(0)> dt$

赤外吸収係数 $\alpha(\omega)$ を計算

$\alpha(\omega) = \frac{4\pi^2}{3hcn} \omega \left\{ 1 - e \times p(- \frac{h\omega}{KT}) \right\} I(\omega)$

IRフルスペクトル計算

END

t=t+Δt

II$_2$

III

【図97】

α-SiO$_2$

300K, 1GPa

ρ =2.34g/cm^3

【図100】

計算セル

フローチャート1 古典的MDを使用して
IRスペクトルを求める場合

入力値の説明図

【図105】

酸化膜

1100℃ドライ酸化10分間

1	酸化膜粘弾性モデル	ON
2	シリコン弾性モデル	ON
3	酸化剤拡散の応力依存性モデル	ON
4	酸化速度の面方位依存性モデル	ON
5	酸化剤/Si反応のSi表面応力依存性モデル	OFF

grid. oxi = 4
init = 0.002分
X方向刻幅 = 10nm

visc. 0 = 2770
visc. e = -2.756
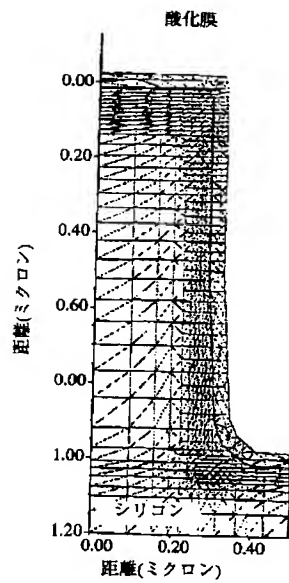
【図１０６】

1100℃ドライ酸化10分間

1	酸化膜粘弾性モデル	ON
2	シリコン弾性モデル	ON
3	酸化剤拡散の応力依存性モデル	ON
4	酸化速度の面方位依存性モデル	ON
5	酸化剤/Si反応のSi表面応力依存性モデル	OFF

grid. oxi = 4
init = 0.15分
X方向刻幅 = 10nm

visc. 0 = 2770
visc. e = -2.756

【図１０７】
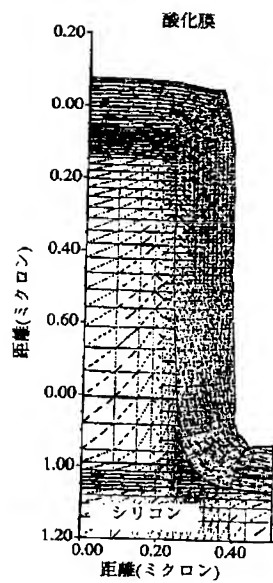
900℃ドライ酸化1000分間

1	酸化膜粘性モデル	ON
2	シリコン弾性モデル	ON
3	酸化剤拡散の応力依存性モデル	ON
4	酸化速度の面方位依存性モデル	ON
5	酸化剤/Si反応のSi表面応力依存性モデル	OFF

grid. oxi = 4
init = 0.002分
X方向刻幅 = 0.5nm
Y方向刻幅 = 0.5nm

visc. 0 = 2770(1倍値)
visc. e = -2.756

【図１０９】

【図１１６】

(a)　　　　　　　　(b)
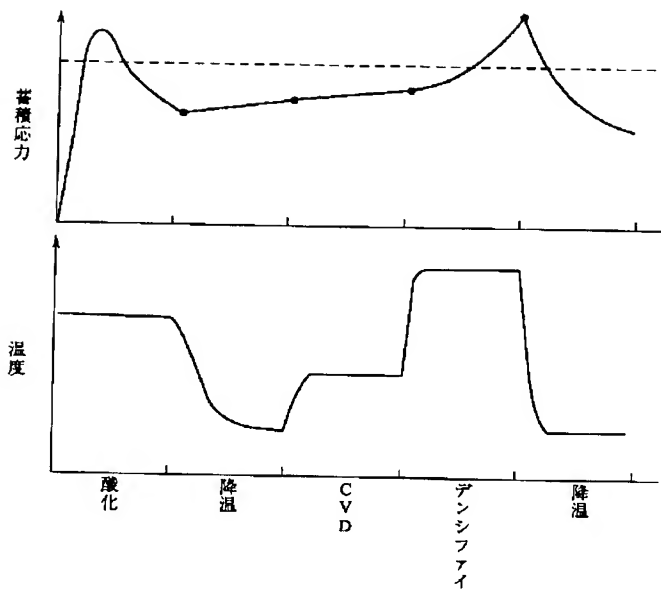
【図１１０】
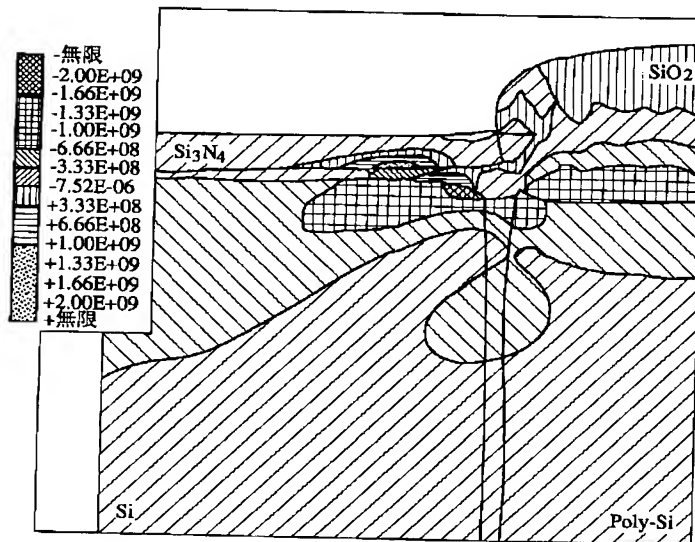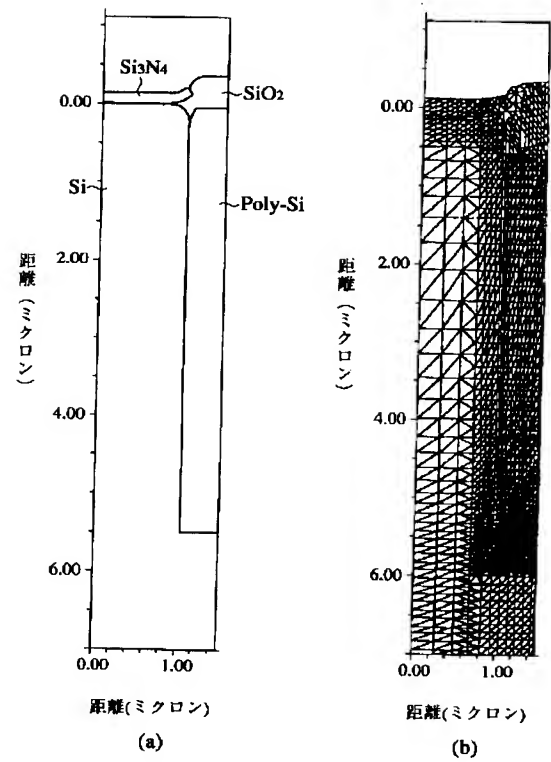
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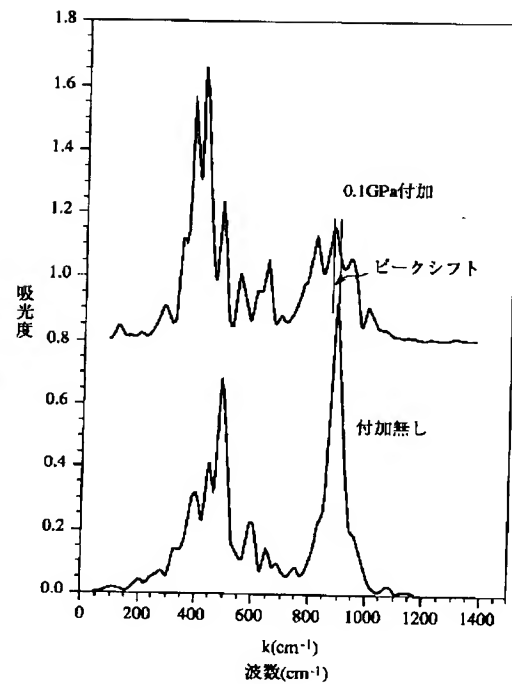
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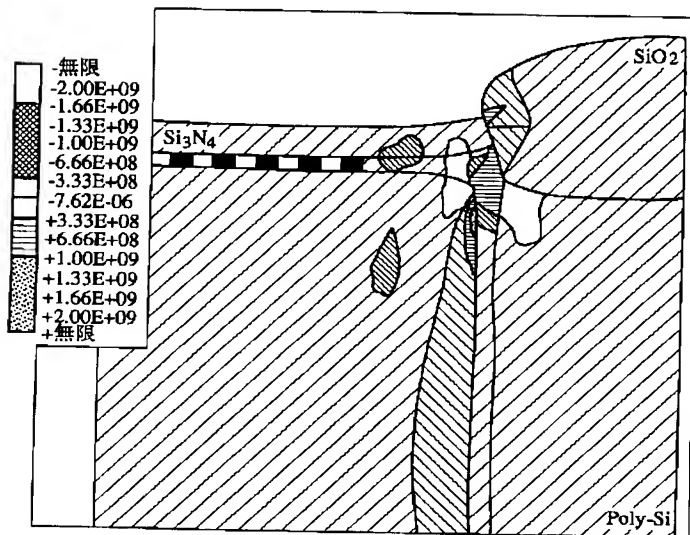
【図112】

【図125】
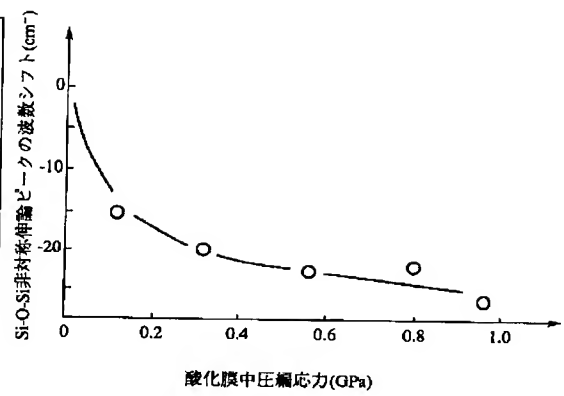
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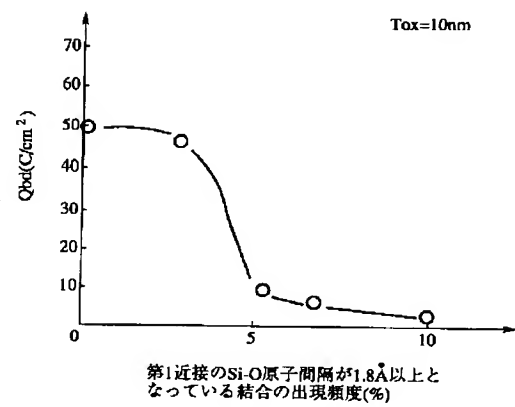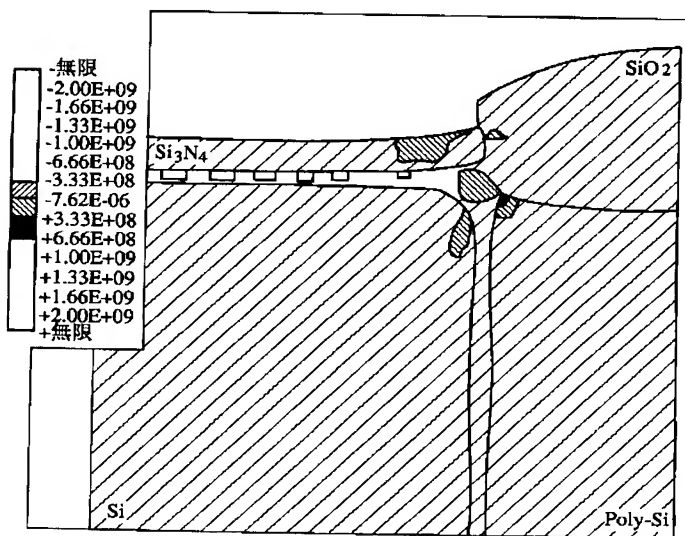
【図130】

クラスタ・ツール
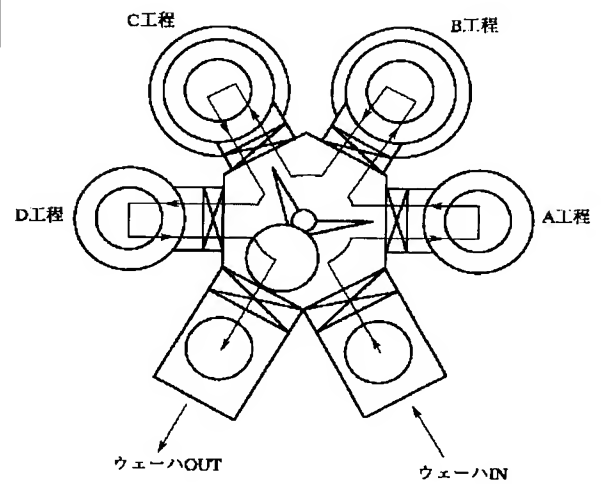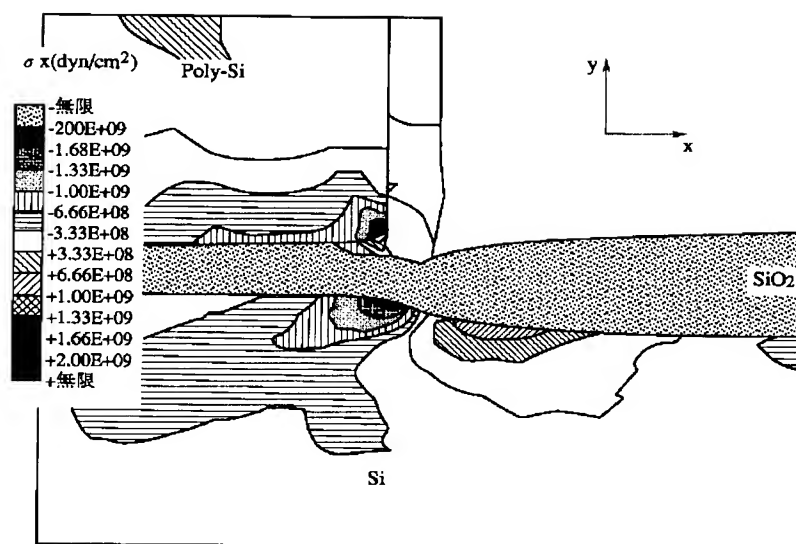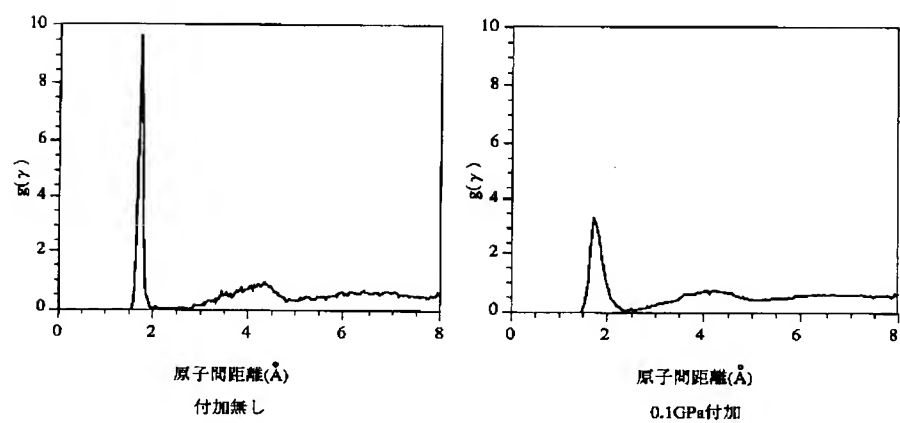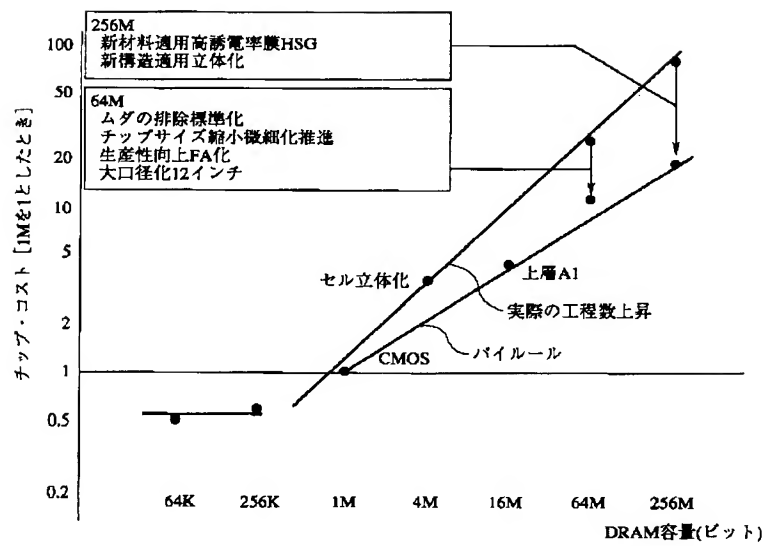
【図１１３】

【図１３１】

【図１１４】

【図１３２】

(A)

(B)
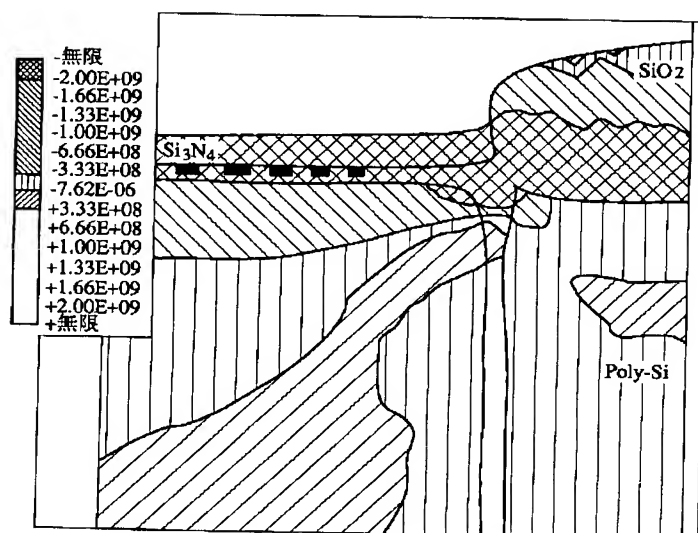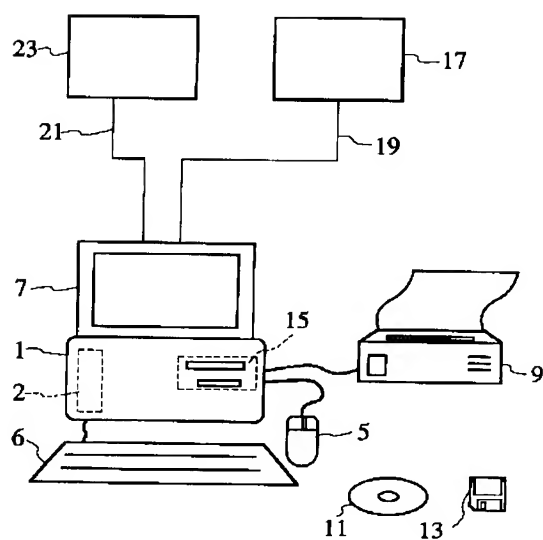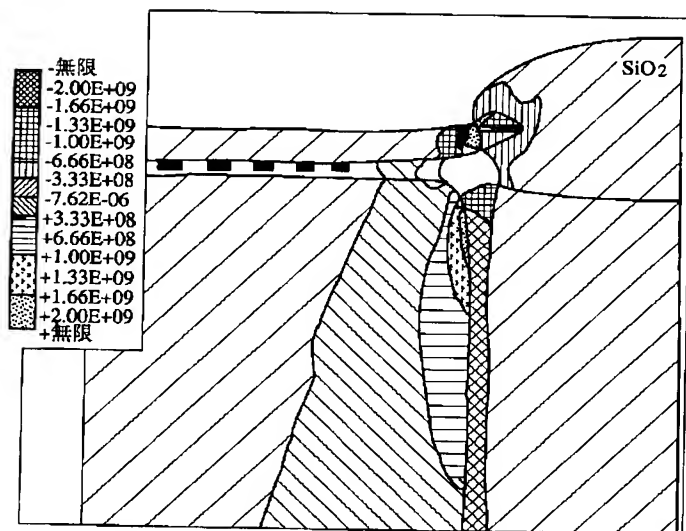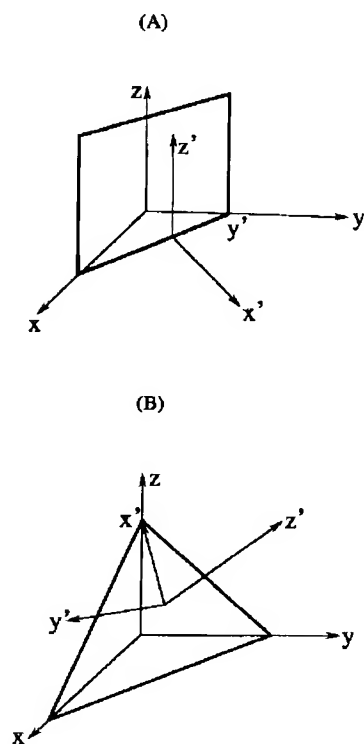
【図１１５】
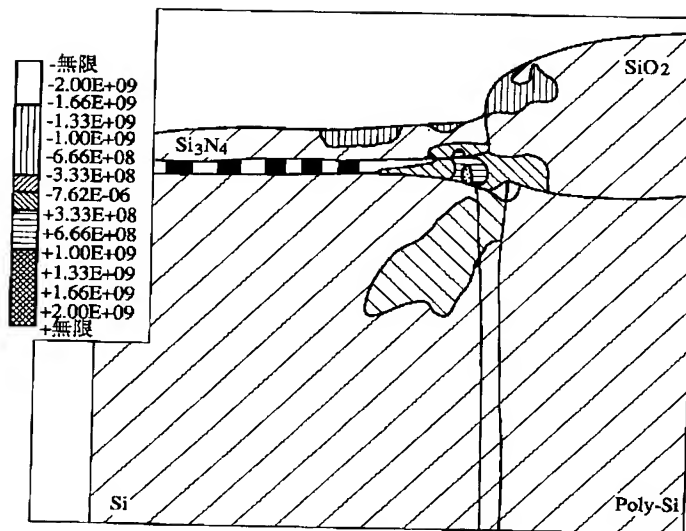
【図１２０】

【図１２１】

【図122】

【図127】

【図128】

【図129】